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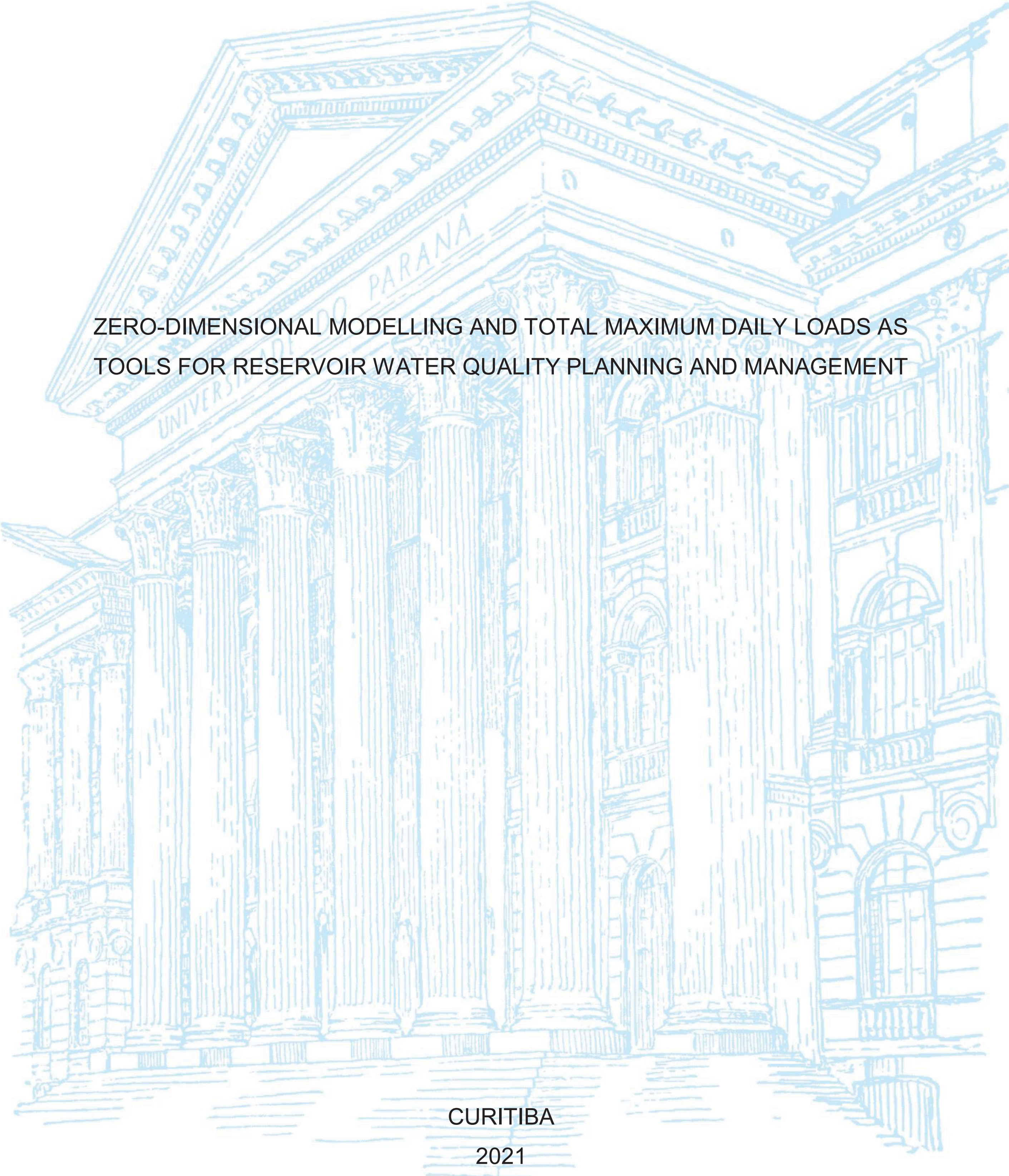
ANA CAROLINA CANOSSA BECKER



ZERO-DIMENSIONAL MODELLING AND TOTAL MAXIMUM DAILY LOADS AS TOOLS FOR RESERVOIR WATER QUALITY PLANNING AND MANAGEMENT

CURITIBA

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Dissertação apresentada como requisito à obtenção do título de Mestre, do Programa de Pós-Graduação em Engenharia de Recursos Hídricos e Ambiental, Setor de Tecnologia, Universidade Federal do Paraná.

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Os membros da Banca Examinadora designada pelo Colegiado do Programa de Pós-Graduação em ENGENHARIA DE RECURSOS HÍDRICOS E AMBIENTAL da Universidade Federal do Paraná foram convocados para realizar a arguição da dissertação de Mestrado de **ANA CAROLINA CANOSSA BECKER** intitulada: **ZERO-DIMENSIONAL MODELLING AND TOTAL MAXIMUM DAILY LOADS AS TOOLS FOR RESERVOIR WATER QUALITY PLANNING AND MANAGEMENT** , sob orientação do Prof. Dr. CRISTOVÃO VICENTE SCAPULATEMPO FERNANDES, que após terem inquirido a aluna e realizada a avaliação do trabalho, são de parecer pela sua APROVAÇÃO no rito de defesa.

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“Individually, we are one drop. Together, we are an ocean.”

- Ryūnosuke Satoro

RESUMO

Modelos de qualidade da água são frequentemente aplicados para apoiar as definições de planejamento e gestão de recursos hídricos. Este processo requer dados apropriados para calibrar e fazer o processo de verificação necessário para análise de validação. No entanto, em alguns estudos de caso, não há dados suficientes para executar um modelo complexo de qualidade da água, seja qual for o sistema de água, seja rio ou reservatório. No contexto de dados escassos, a busca por modelos simples de qualidade da água é uma alternativa para compreender o comportamento da qualidade da água. Nesta pesquisa, um modelo zero-dimensional não-permanente de qualidade de água foi desenvolvido e aplicado utilizando séries sintéticas de concentrações de fósforo para um reservatório brasileiro. Os resultados dos modelos zero-dimensionais desenvolvidos nesta pesquisa foram comparados aos resultados de um modelo tridimensional, a fim de verificar se esta metodologia pode ser uma alternativa mais simples ao modelo tridimensional complexo. Os resultados semelhantes dos modelos zero-dimensional (0D) e tridimensional (3D) mostram que os esquemas numéricos simplificados são importantes ferramentas potenciais a serem consideradas para a análise inicial da dinâmica da qualidade da água em reservatórios e para fins de gestão.

Keywords: Reservatório. Modelo zero-dimensional não permanente. Modelo simplificado.

ABSTRACT

Water quality models are often applied to support the definitions for water resources planning and management. This process requires appropriate data to calibrate and make the required verification process for validation analysis. However, in some case studies, there is not enough data to run a complex water quality model whatever is the water system, being river or reservoir. In the context of scarce data, the search for a simple water quality model is an alternative to comprehend the water quality behavior of the water system. In this research, an unsteady zero-dimensional (0D) water quality model was developed and applied using synthetic series of phosphorus concentrations for a Brazilian reservoir. The results of the zero-dimensional models developed in this research were compared to the results of a three-dimensional water quality model, in order to verify if this methodology can be a simpler alternative to a complex three-dimensional model. The similar results of the zero-dimensional (0D) and three-dimensional (3D) models show the simplified numerical schemes are important potential tools to be considered for initial analysis of water quality dynamics in reservoirs and for management purposes.

Keywords: Reservoir. Unsteady Zero-Dimensional Modelling. Simplified Model.

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1 INTRODUCTION

“We delight in the beauty of the butterfly, but rarely admit the
changes it has gone through to achieve that beauty.”
- Maya Angelou

Reservoirs are built to guarantee distinct water uses, including water and energy supply, recreation activities, fishing and flow regulation. As a consequence, any pollution process can restrict their designated uses. A common cause of pollution is the enrichment of nutrients in the waterbody, which is called eutrophication (ESTEVES, 1998). High concentrations of nitrogen and phosphorus, which come from sewage and agricultural runoff, are responsible for algae blooms and proliferation of aquatic macrophytes (ESTEVES, 1998). Some algae species may present neurotoxic and hepatotoxic effects (HORNE; GOLDMAN, 1994) while macrophytes may cause obstruction of water intakes and increase the organic matter in the water (THOMAZ et al., 2008). Consequently, the water uses may be affected.

In order to maintain the designated uses of a water body, the governmental agencies around the world provide regulation aiming to guarantee the best strategies for water quality planning and management. In Brazil, for instance, the Brazilian Law nº 9.433/1997 (BRASIL, 1997), also known as National Policy of Water Resources, defines five instruments for the water planning and management. One of them is called "Water Quality Classification Framework”, that establishes the overall framework considering the future plans for the watershed, main water uses and the overall reference for future scenarios development. These procedures are regulated by CNRH resolution nº 91/2008 (BRASIL, 2008). This instrument defines the class of a waterbody based on the most restrictive designated use. The CONAMA 357/2005 resolution (BRASIL, 2005) establishes concentration standards for each class of waterbodies, classified according to the legal Water Quality Classification Framework. However, there is no specific methodology for reservoirs water quality classification in the framework context considering that, according to the CNRH resolution nº 91/2008, the Water Quality Classification Framework procedure should consider the specificities of the waterbodies, with emphasis on the lentic environments and the stretches with artificial reservoirs, flow seasonality and intermittent regime. Besides, the general overview of waterbodies based on concentration limits does not allow adequate conditions for analysis considering the dynamics of the water system.

Particularly, in order to improve this Water Quality Classification framework process it is recommended to consider mathematical models that represent physical, chemical and biological processes. Models estimate the performance, in different levels of detail, of numerous set of decisions and assumptions that represent various possible compromises among conflicting groups, values, and management objectives and predict how well the economic, environmental, ecosystem, social or political goals will be met (LOUCKS, BEEK, 2017). They require appropriate data to guarantee the whole traditional requirements for implementation, such as calibration and validation. However, in some situations, there is not enough data to run a complex three-dimensional water quality model. In the context of scarce data, the search for a simple water quality model is an alternative to comprehend the water quality behavior and to assist in defining the Water Quality Classification Framework management recommendations, particularly, for reservoirs.

A potential use for zero-dimensional modelling is the application of this tool in the context of cascading reservoirs, in a way that integrates with a model suitable for rivers. This application would fulfill a gap noticed in river-reservoir integrated studies: the lack of a specific model that includes both environments and properly considers temporal changes, as seen in the theoretical background research (item 2.4).

Another limitation to the adequate assessment of the reservoir environment is that CONAMA 357/2005 Brazilian resolution focus on concentration standards. However, this approach provides a limited understanding of the waterbody behavior, since the same amount of pollution, in mass, may provide different effects on water quality in different flow situations, because the concentration changes as a function of the flow. The United States Environmental Protection Agency (USEPA) provide a different perspective of this problem, determining the calculation of Total Maximum Daily Loads (TMDLs) for impaired waters (USEPA, 2020a). Other regulations indicate following the load analysis tendency, such as Canadian Water Quality Guidelines (CCME, 2021), Australian and New Zealand Guidelines for Fresh and Marine Water Quality (ANZEEC; ARMCANZ, 2000) and European Union Water Framework Directive (EC, 2000).

This research combines the aforementioned aspects of the reservoir planning and management in the case study of the Paranapanema watershed cascade reservoirs, focusing on the zero-dimensional water quality model and using the TMDLs and the river-reservoir integration as complementary aspects of the analysis that aims to contribute to the Water Quality Classification Framework management recommendations. The phosphorus was chosen as model variable since its important behavior limiting the primary productivity of the reservoirs (ANA/UFPR, 2019).

1.1 JUSTIFICATION

The Brazilian current legislation does not properly address procedures for water classification under the perspective of loadings inputs on reservoirs. It may lead to the idea that complex water quality models are always necessary to fulfill this need. However, simplified models can be applied to understand the reservoir water quality. In such context, there is a need for a simplified method to aid the diagnosis of water quality in reservoirs for eventual classification in the Water Quality Classification Framework system. This study case is suitable for the Paranapanema watershed due to its scarce monitoring.

This kind of analysis will be relevant to understand the limitations of the reservoir in terms of capability of receiving load and how such limitations should be reflected in the regulatory legislation. The implementation of this tool in the context of river-reservoir integration models is also an important potential tool for water resources management. Additionally, the TMDL analysis can be helpful to understand the cascade reservoirs capability of receiving load.

1.2 RESEARCH HYPOTHESIS AND OBJECTIVES

The research hypothesis is that the Water Quality Classification Framework strategy can be simplified by means of application of zero-dimensional models on reservoirs, considering spatial and temporal variations. The main goal is the development of a simplified tool to evaluate water quality in reservoirs. The specific goals are:

- **Calculate the Total Maximum Daily Loads**

Determine the loading rate that would be consistent with meeting the Water Quality Criteria (WQC) to the case study reservoirs, which is known as the Total Maximum Daily Load (TMDL) calculation, in order to answer the question: “How much pollution is the reservoir capable of receive without compromising the reservoir planning and management?”.

- **Explore the idea of a river-reservoir integrated model (Model A)**

A simple mathematical modeling program that integrates lotic, lentic and transition environments was developed and denominated “Model A”. The unification of these environments in a single model is an important tool to integrated analysis of the whole watershed. This model is a potential tool to point out the critical locations of the waterbody considering several sectors in order to help on the definition of the Water Quality Classification Framework. The model was applied to Jurumirim reservoir, at the Paranapanema River, Brazil.

- **Develop a simplified zero-dimensional model (Model B)**

A zero-dimensional unsteady water quality model is applied to evaluate the consequences of four different scenarios. This model, indicated as “Model B”, was applied to the three main reservoirs of the Paranapanema watershed (Jurumirim, Chavantes and Capivara).

- **Apply the zero-dimensional model to Jurumirim reservoir sectors (Model C)**

The same zero-dimensional model is applied to the four sectors of Jurumirim reservoir. This configuration was denominated “Model C”.

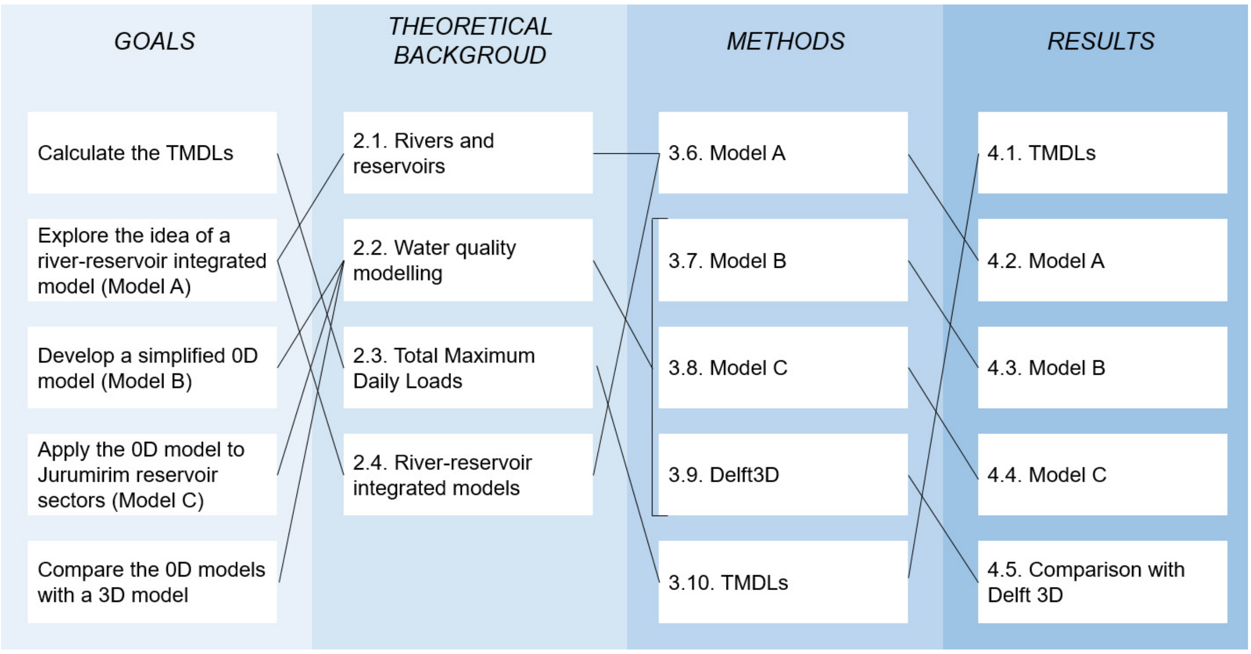
- **Compare the zero-dimensional models with a three-dimensional model**

The results of models B and C were compared to the simulation with the three-dimensional model Delft3D (DELTARES, 2015).

1.3 DOCUMENT ORGANIZATION

The organization of the dissertation document is schematized in Figure 1. The five main goals have their respective chapters in the “Theoretical Background”, “Methods” and “Results” sections.

FIGURE 1 – DOCUMENT ORGANIZATION



2 THEORETICAL BACKGROUND

"If you are the smartest person in the room, then you are in the wrong room"
- Confucius

2.1 RIVERS AND RESERVOIRS

Reservoirs can be built for a variety of reasons, including: water supply, hydroelectric generation, irrigation, flood control, navigation, fishing, and recreation (SCHMUTZ; SENDZIMIR, 2018). According to the authors, the occurrence of environmental impacts is inherent to any impoundment due to changes in hydrology and river morphology.

In rivers, the flow is stronger and driven by gravity down a slope, while in lakes and reservoirs currents are driven by surface winds, buoyancy forces and density currents (CUSHMAN-ROISIN, 2014). Therefore, when a dam is constructed, the lotic environment may turn into lentic environment, which can become stratified and eutrophic.

Depending on the size and shape of the reservoir, a longitudinal hydrological gradient can develop from the dam (lentic environment) to the upstream (lotic environment), demonstrating a gradual hydrological change in characteristics in the intermediate reach, which is characterized by a transition between lentic and lotic features (KIMMEL; GROEGER, 1984 apud SCHMUTZ; SENDZIMIR, 2018).

According to Chin (2006), lentic systems, as reservoirs, lakes and ponds, are more susceptible to pollution when compared to lotic systems, as streams and rivers, which have more tendency to discharge pollutants downstream.

In this context, the nutrient studies along cascade reservoirs are important to prevent the eutrophication process, which is the focus of the present study, despite other possible problems that may affect the reservoir uses.

2.2 WATER QUALITY MODELLING

Von Sperling (2007) claims that modelling is an abstraction, which allows people to concentrate on the essentials of a (complex) problem by keeping out non-essential details for the case study. A model is composed by a theoretical structure (equations), numerical values of the parameters (equations coefficients) and the input and output data.

In cases where the water quality data is scarce, the tendency highlighted in literature is to simplify the models, using less dimensions and considering less processes. In other words, if we do not have water quality data in at least two depths of the reservoir, what would be the representativeness of a three-dimension water quality model focusing on stratification?

Another advantage of the simplified models are the smaller computational time. Therefore, even if the scarce data was not a problem, the 0D models would still be useful depending on the objective of the research conducted or the management purpose. With this in mind, a research about models that use the concept of CSTR (Continuously Stirred Tank Reactor) and zero-dimensional models for simplification was conducted and summarized in Table 1.

Several applications of models simulate river segmented as reservoir compartments, such as Fan et al. (2009), Cox (2003), Karadurmus and Berber (2004), Berber et al. (2009), Keupers and Willems (2017) and Nguyen et al. (2018).

Slaughter et al. (2017) proposed a water quality model that adopts the strategy of modelling reservoirs as a Completely Stirred Tank Reactor (CSTR). The model was able to use the limited observed data to simulate representative frequency distributions of water quality, and the approach used was shown to be suitable for application to data scarce catchments.

Pintilie et al. (2007) also applied a zero-dimensional model considering the mass balance and complementary equations for metals, under several scenarios with steady conditions. Also, Toné (2016) applied and calibrated the CSTR model to 33 reservoirs of Brazil's northeast semiarid region and validates the model with data from 8 reservoirs of the South African semiarid.

Polli (2018) also followed the simplification tendency. The author divided a reservoir in sectors and applied Delft3D model in a simplified configuration. That research showed it was possible to identify periods of mixing and stratification with simple models and low time processing.

None of the evaluated models considered the atmospheric deposition and only five of the 13 researches evaluated in Table 1 considered internal loading contributions. For this reason, those processes were not considered in the present research.

TABLE 1 – MODELS THAT USE THE CONCEPT OF CSTR (CONTINUOUSLY STIRRED TANK REACTOR) FOR SIMPLIFICATION

Title	Authors	What did they do?	Model	Variables modelled	Internal loading?	Steady?	Equation
Development and testing of a fast conceptual river water quality model	Keupers; Willems (2017)	Developed a water quality model for rivers divided into conceptual reservoirs. These reservoirs are modelled as Plug Flow Reactor (PFR) and Continuously Stirred Tank Reactor (CSTR).	Plug Flow Reactor (PFR) and as a Continuously Stirred Tank Reactor (CSTR)	Dissolved Oxygen (DO), Biological Oxygen Demand (BOD), ammonia (NH4), nitrate (NO3), orthophosphate (OP), particulate phosphorus (PP) and temperature (T)	Yes	Steady	$C_{out,AD}(t) = exp\left(\frac{-1}{k}\right)C_{out}(t-\Delta t) + \left[1 - exp\left(\frac{-1}{k}\right)\right]C_{in}(t-\delta)$
A management-oriented water quality model for data scarce catchments	Slaughter et al. (2017)	Proposes a water quality model that adopts the strategy of modelling reservoirs as a completely stirred tank reactor (CSTR). The model was able to use the limited observed data to simulate representative frequency distributions of water quality, and the approach used was shown to be suitable for application to data scarce catchments.	WQSAM	Salinity and nutrient concentrations	Yes	Unsteady	Not available
An innovative modeling approach using Qual2K and HEC-RAS integration to assess the impact of tidal effect on River Water quality simulation	Fan; Ko; Wang (2009)	Combines the Qual2K model with the HEC-RAS model to assess the water quality of a tidal river	Qual2K with HEC-RAS	biochemical oxygen demand (BOD), ammonia nitrogen (NH3-N), total phosphorus (TP), and sediment oxygen demand (SOD)	No	Unsteady	$\frac{dC_i}{dt} = \frac{Q_{i-1}}{V_i}C_{i-1} - \frac{Q_i}{V_i}C_i - \frac{Q_{out,i}}{V_i}C_i + \frac{E_{i-1}}{V_i}(C_{i-1} - C_i) + \frac{E_i}{V_i}(C_{i+1}C_i) + \frac{W_i}{V_i} + S_i$
Dynamic simulation and parameter estimation in river streams	Karadurmus; Berber (2004)	A dynamic model based on QUAL2E was introduced. The basic assumption was that a river reach could be modeled as a single CSTR.	CSTR (based on QUAL2E)	ammonia, nitrite, nitrate, organic nitrogen, organic phosphorus, dissolved phosphorus, biological oxygen demand (BOD), dissolved oxygen, coliforms, chloride and Chlorophyll-a	No	Unsteady	$\frac{dN_1}{dt} = [-\beta_1 \cdot- (Q/V)]\,N_1 - [F_1 \cdot \alpha_1 \cdot \mu \cdot]\,A + [\delta_3/d + (Q/V)\,N_1^0]$
A parameter identifiability and estimation study in Yesilirmak River	Berber; Yuceer; Karadurmus (2009)	A river reach is represented by a series of CSTRs rather than a single one.	CSTR (based on QUAL2E)	Organic nitrogen, ammonia nitrogen, nitrite nitrogen, nitrate nitrogen, biochemical oxygen demand, dissolved oxygen, organic phosphorus, dissolved phosphorus, coliforms, chloride, planktonic algae.	No	Steady	$\frac{dN_1}{dt} = [-\beta_1 \cdot- (Q/V)]\,N_1 - [F_1 \cdot \alpha_1 \cdot \mu \cdot]\,A + [\delta_3/d + (Q/V)\,N_1^0]$
A review of currently available in-stream water-quality models and their applicability for simulating dissolved oxygen in lowland rivers	Cox (2003)	A review is undertaken of the major models currently in use for describing water quality in freshwater river systems. These models have been developed for particular purposes and this review shows that no one model can provide all of the functionality required.	**SIMCAT, TOMCAT,** QUAL2E, QUASAR, MIKE-11 and ISIS	Dissolved Oxygen (DO)	No	Steady	SIMCAT: $\frac{dC}{dt} = -K_r L + K_a(C_s - C)$ TOMCAT: $\frac{dC}{dt} = K_a(C_s - C) - \frac{dL}{dt} - 4.57\frac{d[NH_4]}{dt}$
Conceptual river water quality model with flexible model structure	Nguyen; Keupers; Willems (2018)	The model conceptualizes rivers using cascades of reservoirs	CORIWAQ	Dissolved Oxygen, organic matter, nitrogen and phosphorus	No	Unsteady	$c_{out}(t) = e^{-\frac{1}{k}}\,c_{out}(t-\Delta t) + \left[1 - e^{-\frac{1}{k}}\right]\,c_{in}(t-\delta) + \frac{\Delta c}{\Delta t}(k+\delta)$
Modelling and simulation of heavy metals transport in water and sediments	Pintilie et al. (2007)	Metals transport and sedimentation is simulated based on an analytical model proposed in literature, considering the material balance and complementary equations, under dynamic conditions	Mass balance and complementary equations	Metals	Yes	Steady	$\frac{dC_{T_1}}{dt} = Q(C_{in} - C_{T_1}) - \frac{v_s}{H_1}(1-f_D)C_T - \frac{K_1}{H_1}(C_{D_1} - C_{D_2})$ $\frac{dC_{T_2}}{dt} = \frac{v_{s_1}}{H_2}(1-f_{D_1})C_{T_1} + \frac{K_L}{H_2}(C_{D_1} - C_{D_2}) - \frac{v_{s_2}}{H_2}(1-f_{D_2})C_{T_2}$
Simple modelling of total phosphorus in brazilian lakes and reservoirs	Toné; Lima Neto (2020)	Total mixed model to analyze de phosphorus dynamics in 40 reservoirs and lakes.	Vollenweider (1968)	Total phosphorus	No	Unsteady	$V\frac{dP}{dt} = W - QP - kVP \qquad P = P_o e^{-\lambda t} + \frac{W}{\lambda V}\left(1 - e^{-\lambda t}\right)$
Modelling the impact of sediment management on the trophic state of a tropical reservoir with high water storage variations	Lira; Medeiros; Lima Neto (2020)	An assessment of the impact of the silted sediment management on the trophic status of a tropical surface reservoir with intense temporal variability of water storage. A complete mixing model describing the total phosphorus budget in the water and sediments was used, based on semi-empirical formulations.	Chapra and Canale (1991); Vollenweider (1976)	phosphorus	Yes	Unsteady	$V_1\frac{dp_1}{dt} = W - Qp_1 - v_s A_2 p_1 + v_r A_2 p_2$ $V_2\frac{dp_2}{dt} = v_s A_s p_1 - v_r A_2 p_2 - v_b A_2 p_2$

Title	Authors	What did they do?	Model	Variables modelled	Internal loading?	Steady?	Equation
Impact of flow conditions on coliform dynamics in an urban lake in the Brazilian semiarid	Fraga; Rocha; Lima Neto (2020)	Considering both the plug-flow and complete-mix models, it was shown that eliminating dry weather load reduces total coliforms and Escherichia coli but still leads to exceedances of the mandatory standards during the rainy season.	steady-state plug-flow model, complete-mix model, transient complete-mix model	total coliforms and Escherichia coli	No	Steady and unsteady	$C = C_o.e^{-kx/u}$ (steady−state plug−flow model) (1) $C = Q_oC_o/(Q + kV)$ (steady−state complete−mix model) (2) $C_{i+1} = V_iC_i(1-k\Delta t)/V_{i+1}$ (transient complete − mix model) (9)
Removal of organic matter in stormwater ponds: a plug-flow model generalization from waste stabilisation ponds to shallow rivers	Araújo; Lima Neto (2019)	This study investigates the effect of flow conditions on the organic matter concentration, removal efficiency, and reaction kinetics in a stormwater pond. The best fit was achieved considering the plug-flow assumption, and a general BOD model. Simulations with this general model were performed to assess the impact of remediation measures on the studied pond.	plug-flow	biochemical oxygen demand (BOD) and chemical oxygen demand (COD)	No	Steady	$C = C_0.e^{-kt}$ (plug − flow model) (1) $C = C_0/(1 + kt)$ (complete − mix model) (2)
Phosphorus dynamics in a highly polluted urban drainage channel-shallow reservoir system in the Brazilian semiarid	Araújo; Lima Neto; Becker (2019)	Quantify non-point source phosphorus loads along the channel from residences unconnected to sewers, investigate the flow conditions and their impacts on phosphorus dynamics, and adjust phosphorus decay coefficients for both the channel and the reservoir, and compare the results with those available in the literature for non-semiarid regions.	Chapra (2008)	phosphorus	Yes	Steady	$P = P_0 e^{-\left(\frac{Q}{V}+k_r\right)t} + \frac{W}{(Q+k_rV)}\left[1-e^{-\left(\frac{Q}{V}+k_r\right)t}\right]$

2.3 TOTAL MAXIMUM DAILY LOADS (TMDL)

According to USEPA (2020a), a Total Maximum Daily Load (TMDL) is the maximum amount of a pollutant allowed to enter a waterbody so that it will still respect the water quality standards for that particular pollutant.

The TMDL was established by the Clean Water Act. The Federal Water Pollution Control Act was created in 1948 and was reorganized and expanded in 1972, when it became known as the “Clean Water Act”. This regulation establishes how to plan actions aiming the restoration of impaired waters. When the water is recognized as “impaired”, it is required to the relevant entity to access and allocate pollutant loads in a manner that the Water Quality Standards are attained (USEPA, 2020b).

USEPA (2020b) explains that the TMDL process is divided into two main steps: the first one is quantifying existing pollutant loads and the second is calculating the load reductions needed to meet the Water Quality Standards. Besides, the aforementioned report also highlights three elements of a TMDL:

1) **Acceptable load (pollutant cap):** is the loading rate that would meet the Water Quality Criteria.
2) **Margin of Safety (MOS):** is an extra measure of protection, which takes into account the uncertainties of the loading rate calculation.
3) **Allocation of the acceptable load among sources:** is the distribution of the loading rate between the sources in a manner that Water Quality Standards are achieved.

Table 2 shows examples of how TMDL has been explored in literature. There is no doubt of the relevance of TMDL concept and its understanding as tool for water resources planning and management strategies. Additionally, the use of modelling tools is consolidated as well using the same approach. However, the integration tools for emission loads, river impacts and reservoir responses that consider temporal dynamics still requires more in-depth understanding and complementary computer tools. This research establishes the first element (acceptable load) and compares with the zero-dimensional model results.

TABLE 2 – TOTAL MAXIMUM DAILY LOAD (TMDL) APPLICATIONS

Article	Authors	Journal	Year	Country	What did they do?	What's the conclusion?
Water quality decisions and policy for an interstate watershed	Fernandez; McGarvey	Water Resources and Economics	2019	USA	They develop and apply a dynamic game model with economic, hydrologic, environmental and institutional components for interdependent states to reach the Total Maximum Daily Load (TMDL) water quality goals either jointly or separately. It´s an economic tool for P abatement across transboundary emitters at least coast to meet a TMDL water quality goal.	Comparing noncooperation and cooperation based on three different sector's abatement cost functions in different states, helps to delineate key differences in the amount of P reduction and the frequency in meeting water quality goals of total P load reduction to accomplish the water quality regulation goal for the time horizon.
Modeling nitrogen transport in the Newport Bay/San Diego Creek watershed of Southern California	French; Wu; Meixner; Haver; Kabashima; Jury	Agricultural Water Management	2006	USA	The Newport Bay/San Diego Creek watershed has had a total maximum daily load (TMDL) established for the allowable loading of nitrogen into the bay. Baseline allocations for the TMDL indicate that 30% of the total nitrogen load is from agriculture; however, observations from a monitoring study and estimates from a conceptual model show that nitrogen from agriculture contributions is more likely between 2 and 8% of the total.	Nutrient contributions from agricultural sites are likely to become even less important over the coming years as more agricultural land is converted to urban use.
Planning for water quality in OH: What role(s) for planners?	Conroy	Environmental Science and Policy	2018	USA	This paper uses the state of Ohio as a case study to explore the role of planning and planners with respect to nonpoint source water quality mitigation, specifically related to the Section 319 grant related funding, through watershed planning efforts. Section 319 directed watershed planning are focused on TMDL guidelines to combat nonpoint source pollution levels.	Planners are not involved enough in water decisions, because of the lack of integration between water quality and TMDL goals and the other government plans, such as land use
Bayesian approach to estimating margin of safety for total maximum daily load development	Patil; Deng	Journal of Environmental Management	2011	USA	A Bayesian-updating approach is presented to the estimation of total uncertainty-based Margin of Safety (MOS) for Total Maximum Daily Load (TMDL) calculations.	This newly developed probabilistic method was found to be more reliable and inclusive of different sources of uncertainties.
A procedure for setting environmentally safe total maximum daily loads (TMDLs) for selenium	Lemly	Ecotoxicology and Environmental Safety	2002	USA	There is no technical guidance from EPA or elsewhere that deals exclusively with selenium. This article provides guidance by laying out an assessment method that links the basic components of EPA's TMDL process to the contaminant-specific information required for selenium.	The HU (hydrological unit) approach provides the contaminant-specific site characterization that is necessary for selenium. Proper application of this TMDL technique will ensure compliance with EPA regulatory requirements and also protect fish and wildlife resources.
Use of continuous and grab sample data for calculating total maximum daily load (TMDL) in agricultural watersheds	Gulati; Stubblefield; Hanlon; Spier; Stringfellow	Chemosphere	2014	USA	The objective was to compare the accuracy of five load estimation methods to calculate pollutant loads from agricultural watersheds	The results show that parametric methods are surprisingly accurate, even for data that have starkly non-normal distributions and are highly skewed
A framework for uncertainty and risk analysis in Total Maximum Daily Load applications	Camacho; Martin; Wool; Singh	Environmental Modelling and Software	2018	USA	TMDL studies rarely include an explicit uncertainty analysis and the estimation of the MOS is often subjective and even arbitrary. A Bayesian framework to compute TMDLs and MOSs including an explicit evaluation of uncertainty and risk is proposed.	The formulation of a TMDL as a problem of risk of non-compliance is the basis for a more objective and convenient approach to set the goals of the TMDL and to define the MOSs.

Article	Authors	Journal	Year	Country	What did they do?	What's the conclusion?
Development and application of mathematical models to support total maximum daily load for the Taihu Lake's influent rivers; China	Wang; Bi; Ambrose	Ecological Engineering	2015	China	A site specific empirical model is developed and linked to a general, mechanistic model of water quality.	The model performs satisfactorily for prediction of pollutant fate and evaluation of various modeling scenarious to meet the target TMDL condition. The calculated TMDL reductions can provide a scientific basis for the authority to make water pollution management decisions.
Development of a total maximum daily load (TMDL) for acid-impaired lakes in the Adirondack region of New York	Fakhraei; Driscoll; Selvendiran; DePinto; Bloomfield; Quinn; Rowell	Atmospheric Environment	2014	USA	A biogeochemical model was used to relate decreases in atmospheric sulfur and nitrogen deposition to changes in lake water chemistry.	The TMDL of acidity corresponding to a moderate control scenario was estimated, including a 10% MOS.
The importance of considering biological processes when setting total maximum daily loads (TMDL) for phosphorus in shallow lakes and reservoirs	Havens; Schelske	Environmental Pollution	2001	USA	Considers how biological processes can influence the ability of lakes to assimilate P, and in turn the ability of managers to select appropriate TMDLs.	If some biological changes can be reversed in a rehabilitation program then the lake may be able to support a higher TMDL.
Watershed model calibration framework developed using an influence coefficient algorithm and a genetic algorithm and analysis of pollutant discharge characteristics and load reduction in a TMDL planning area	Cho; Lee	Journal of Environmental Management	2015	South Korea	A calibration framework is developed using an influence coefficient algorithm and genetic algorithm to calibrate the models. The pollution discharges from the watershed were estimated for each land-use type, and the seasonal variation of the pollution loads were analyzed. The exceedance frequency of the water quality standard was calculated for each hydrologic condition class, and the percent reduction required to achieve the water quality standard was estimated.	The critical conditions for TP occur under high-flow conditions, wherein a 66% loading reduction is required to meet the WQS. These reductions could represent goals to work towards in the implementation phase of the TMDL process.
An integrated environmental decision support system for water pollution control based on TMDL - A case study in the Beiyun River watershed	Zhang; Li; Zhang; Peng	Journal of Environmental Management	2015	China	An Environment Decision Support System (EDSS) was developed to establish a daily water quality simulation, maximum daily load calculation and pollutant load reduction measures simulation using water environment management based on TMDL.	The integration is easy to implement and enables different development languages and reuse of existing models.
Applying SWAT for TMDL programs to a small watershed containing rice paddy fields	Kang; Park; Lee; Yoo	Agricultural Water Management	2006	USA	Apply the soil and water assessment tool (SWAT) to develop TMDL programs.	The total maximum daily load system (TOLOS) appears to be a useful tool for planning TMDL for a small watershed.
Impacts of a thermal power plant on the phosphorus TMDL of a reservoir	Chen; Weintraub; Herr; Goldstein	Environmental Science and Policy	2000	USA	The Watershed Analisys Risk Management Framework (WARMF) was applied to calculate the TMDL of total phosphorus discharged to a reservoir without violating the water quality criteria of chlorophyll-a.	The TMDL of phosphorus was higher with a thermal power plant than without. Policy makers can learn, through this type of scientific analysis, about the impacts of a thermal power plant and make rational decisions about phosphorus TMDL.
Risk-based decision making to evaluate pollutant reduction scenarios	Ahmadisharaf; Benham	Science of the Total Environment	2020	USA	Presents a risk-based framework for evaluating alternative pollutant allocation scenarios considering reliability in achieving water quality goals.	Achieving water quality goals with very high reliability was not possible, even with extreme levels of pollutant reduction.

Article	Authors	Journal	Year	Country	What did they do?	What's the conclusion?
Three-dimensional hydrodynamic and water quality model for TMDL development of Lake Fuxian; China	Zhao; Zhang; Liu; He; Zhu; Zou; Zhu	Journal of Environmental Sciences (China)	2012	China	The TMDL was calculated using two interpretations of the water quality standards for Class I of the China National Water Quality Standard (CNWQS) based on the maximum instantaneous surface and annual average surface water concentrations.	The model results show that, under the existing conditions, the average water quality meets the Class I standard and therefore load reduction is unnecessary.
A Bayesian changepoint-threshold model to examine the effect of TMDL implementation on the flow-nitrogen concentration relationship in the Neuse River basin	Alameddine; Qian; Reckhow	Water Research	2011	USA	Most adopted models assume that the relationship between flow and concentration is fixed across time as well as across different flow regimes. In this study, we developed a Bayesian changepoint-threshold model that relaxes these constraints and allows for the identification and quantification of any changes in the underlying flow concentration relationship across time.	The results from our study support the occurrence of a changepoint in time around the year 1999, which coincided with the period of implementing nitrogen control measures as part of the TMDL program developed for the Neuse Estuary in North Carolina.
Ranking tributaries for setting remediation priorities in a TMDL context	Stringfellow	Chemosphere	2008	USA	Nonparametric methods based on ranking were used to compare the WQ of individual tributaries and drainages. Normalized rank means (NRMs) were calculated from ranked data and NRMs were mapped to identify priority drainages for WQ improvement activities. NRMs for individual parameters were combined into indexes that are useful for examining the relative importance of different drainages for multiple parameters simultaneously. Indexes were developed for eutrophication and overall WQ. Comparative methods are obviously useful tools for the TMDL process.	This ranking approach is being proposed as an easily understood, transparent, and scientifically rigorous method to assess the relative WQ impact of individual drainages and set watershed remediation priorities.
A Bayesian approach for evaluation of the effect of water quality model parameter uncertainty on TMDLs: A case study of Miyun Reservoir	Liang; Jia; Xu; Xu; Melching	Science of the Total Environment	2016	China	An allowable pollutant load calculation platform was established using the Environmental Fluid Dynamics Code (EFDC),which is a widely applied hydrodynamic-water quality model. A Bayesian approach was applied to assess the effects of parameter uncertainty on the water quality model simulations and its influence on the allowable pollutant load calculation in the TMDL program.	The wide ranges of allowable pollutant loads reveal the importance of parameter uncertainty analysis in a TMDL program for allowable pollutant load calculation and margin of safety (MOS) determination. The sources of uncertainty are discussed and ways to reduce the un- certainties are proposed.

2.4 RIVER-RESERVOIR INTEGRATED MODELS

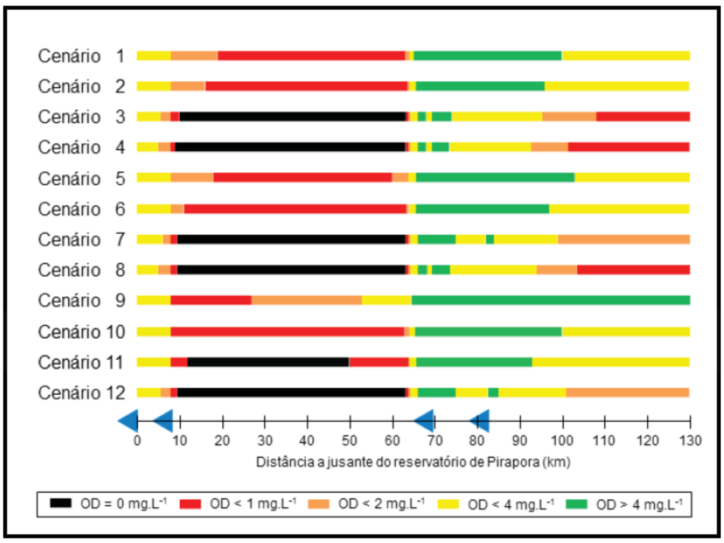
Many studies that integrate rivers and reservoir focused on sediment transport, such as the ones presented by Feng et al. (2019), Guo et al. (2020), Alighalehbabakhani et al. (2017) and Li et al. (2018).

Guo et al. (2020) explored the impacts of cascade reservoirs on the grain size and mineral composition of fine sediments. Alighalehbabakhani et al. (2017) evaluated the sediment accumulation rates of twelve reservoirs within the Great Lakes watershed using the Soil and Water Assessment Tool (SWAT). Based on the sediment accumulation rate, the remaining reservoir capacity for each study site was estimated. Li et al. (2018) indicated that human activities, in particular cascade damming, played a predominant role in sediment load changes, while climate variations mainly impacted discharge changes in the evaluated basin.

Studies focusing on water quality along river-reservoir systems are also being produced. The following authors can be cited as examples:

Tercini and Méllo Júnior (2016) applied Streeter-Phelps basic equations in order to model the BOD (Biochemical Oxygen Demand) and DO (Dissolved Oxygen) concentrations along the Tietê river passing through four reservoirs: Pirapora, Rasgão, São Pedro e Porto Góes. The authors modeled 12 scenarios, in which the discharge, level and affluent BOD in the system varied. As a result of the aforementioned study, the concentrations of DO along the river were estimated, passing through four reservoirs (represented by blue triangles in Figure 2). This model indicated that the critical reach for the dissolved oxygen would be between the Rasgão (kilometer 10) and São Pedro (kilometer 70) reservoirs.

FIGURE 2 – DISSOLVED OXYGEN CONCENTRATIONS ESTIMATED BY STREETER-PHELPS MODEL



SOURCE: TERCINI; JÚNIOR (2016)

Cunha-Santino et al. (2017) applied a steady zero-dimensional model, in order to model 23 limnologic variables in a system of six cascade reservoirs. They concluded that the six reservoirs were very efficient in retaining elements, which emphasized the role of these reservoirs for the mitigation of eutrophication, turbidity, total solids, color and coliforms of the Juquiá-Guaçu river.

Kerachian and Karamouz (2007) developed optimal operation rules for a river-reservoir system aiming water quality management, considering the temperature and total dissolved solids. Wang et al. (2016) modeled the water quality and quantity of a cascade reservoir-system as well, in order to analyze the effects of current and future water diversion projects. Long et al. (2019) analyzed the alteration of discharge and water temperature caused by two newly established cascade reservoirs, using CE-QUAL-W2 two-dimensional model.

Che and Mays (2015) presented the development and testing of a methodology for determining reservoir release schedules before, during, and after an extreme flood event in real time. However, Che and Mays (2015) considered only water quantity. Water quality and quantity in a common management strategy were considered in a multi-reservoir optimization model by Sechi and Sulis (2009). These references justify the inclusion of the water quantity dynamics in the models presented further in this study.

Chen et al. (2018) investigated the distribution and composition of pesticides along the environmental gradient from upstream river system to downstream reservoir system, which was considered as a hybrid river-reservoir system. The perspective of the study, considering the hydrological gradient, led to the identification of the distributions and environmental behavior of pesticides in river-reservoir system. It was found that they varied seasonally from river system to reservoir system.

Chen et al. (2019) presented an approach that couples multiobjective reservoir operation optimization with dynamic mass balance calculation of total phosphorus. They concluded that total phosphorus export from the evaluated river is closely related to characteristics of the cascade reservoirs, including the storage capacity and residence time of the reservoirs, as well as their locations.

Jurczak et al. (2019) aimed to verify the improvement of the water quality after restoration of a small, stormwater-fed urban river and a cascade of ponds and reservoirs. They showed that four years after restoration, the concentrations of the total forms of nutrients and ammonium were still considerably lower than before restoration.

Morales-Marín et al. (2017) identified the major nutrient sources and quantification of nutrient export from the catchment at different spatial scales. Model results indicate that evaluated lake retains about 70% of the inflowing total nitrogen (TN) and 90% of the inflowing total phosphorus (TP) loads.

Chen; Chong; Li (2021) adopt the Hydrological Simulation Program-FORTRAN (HSPF) and the Water Quality Analysis Simulation Program (WASP) as combined tools to model phosphorus concentrations in a reservoir. This study demonstrated the usage of this tool could guide effective catchment management and eutrophication risk prevention.

The studies cited above are summarized in Table 3. This research complement these understandings by considering a 0D water quality model for management purposes adding temporal dynamics under scarce water quality database.

TABLE 3 – RIVER-RESERVOIR INTEGRATED MODELS

Article	Authors	Journal	Year	Country	What did they do?	Variables modelled
Simulation model of DO and BOD integrating river and reservoir applied to the Tietê River	Tercini; Méllo Júnior	Revista Brasileira de Recursos Hídricos	2016	Brazil	A simulation model of DO and BOD combining rivers and reservoirs was developed	Dissolved Oxygen, Biochemical Oxygen Demand
A stochastic conflict resolution model for water quality management in reservoir–river systems	Kerachian; Karamouz	Advances in Water Resources	2007	Iran	Optimal operating rules for water quality management in reservoir–river systems are developed using a methodology combining a water quality simulation model and a stochastic GA-based conflict resolution technique.	Water temperature and Total Dissolved Solids (TDS)
Modelling water quality and quantity with the influence of inter-basin water diversion projects and cascade reservoirs in the Middle-lower Hanjiang River	Wang; Zhang; Zhao; Peng; Shi	Journal of Hydrology	2016	China	Proposes a 1D hydrodynamic model with water-quality model to analyze the effects of current and future inter-basin water diversion projects	COD, NH4, TP
Effect of Cascading Reservoirs on the Flow Variation and Thermal Regime in the Lower Reaches of the Jinsha River	Long; Ji; Liu; Yang; Lorke	Water	2019	China	Analyzed the alteration of discharge and water temperature caused by two newly established reservoirs	Discharge and water temperature
Development of an Optimization/Simulation Model for Real-Time Flood-Control Operation of River-Reservoirs Systems Sustainability Assessment for the Long-Term Transition of Urban Water Supply Systems View project Modeling (rainfall-runoff, river, reservoir) View project	Che; Mays	Water Resources Management	2015	USA	This paper presents the development and testing of a methodology for determining reservoir release schedules before, during, and after an extreme flood event in real time.	Flow
A modeling approach for a cascade of reservoirs in the Juquiá-Guaçu River (Atlantic Forest, Brazil)	Cunha-Santino; Fushita; Bianchini	Ecological Modelling	2017	Brazil	Based on a zero-dimensional model, this work describes the mass balances of 23 limnological variables in a system of 6 cascade reservoirs.	DO, pH, TS, COD, Alkalinity, TC, DIC, DOC, TP, TDP, TPP, N-NO3, N-NO2, N-NH4, N-Org, TIN, TN
Dynamic attribution of water quality indexes in a multi-reservoir optimization model	Sechi; Sulis	Desalination	2009	Italy	A simplified approach that includes water quality aspects as water use limiting factors in a multi-reservoir optimization model can be achieved by adoption of the Trophic State Index (TSI). The application of the optimization approach to different operating rules in a real multi-reservoir system in southern Sardinia highlights the need for joint consideration of quality and quantity aspects for effective water management.	Chlorophyll-a
Occurrence, distribution and risk assessment of pesticides in a river-reservoir system	Chen; Yu; Hassan; Xu; Zhang; Gin; He	Ecotoxicology and Environmental Safety	2018	China	Illustrates the occurrence, distribution, ecological risk of the pesticides in the water phase of Headwater Region of the Dongjiang River, and systematically investigates their distribution and composition along the environmental gradient from upstream river system to downstream reservoir system	31 target pesticides

Article	Authors	Journal	Year	Country	What did they do?	Variables modelled
Influence of dam reservoir on the water quality in a small upland river	Zubala	Ecohydrology and Hydrobiology	2009	Poland	Evaluates the functioning possibilities of small dam reservoir localized within eroded agricultural catchment – namely its interaction with the river water quality. Changes of selected chemical variables and some physical parameters of water at three control points (inflow, reservoir and outflow) have been assumed as criteria of assessment.	temperature, electrolytic conductivity, pH, total suspension, dissolved oxygen, BOD5, COD, ammonia, nitrates, nitrites, phosphates, sulfates, iron, potassium, chlorides.
Nexus of water; energy and ecosystems in the upper Mekong River: A system analysis of phosphorus transport through cascade reservoirs	Chen; Xu; Zheng; Zhang	Science of the Total Environment	2019	China	This study develops a system modeling approach to address the water-energy-ecosystem (WEE) nexus associated with the operation of cascade reservoirs. The approach couples multiobjective reservoir operation optimization with dynamic mass balance calculation of total phosphorus (TP).	total phosphorus
Comprehensive approach to restoring urban recreational reservoirs. Part 1 – Reduction of nutrient loading through low-cost and highly effective ecohydrological measures	Jurczak; Wagner; Wojtal-Frankiewicz; Frankiewicz; Bednarek; Łapińska; Kaczkowski; Zalewski	Ecological Engineering	2019	Poland	The study presented in this paper aimed to improve the water quality of a small, stormwater-fed urban river and a cascade of ponds and reservoirs. A combination of conventional restoration methods and comprehensive ecohydrological restoration methods was tested.	total nitrogen, total phosphorous, nitrate, phosphate, ammonium, total suspended solids
Assessment of nutrient loadings of a large multipurpose prairie reservoir	Morales-Marín; Wheater; Lindenschmidt	Journal of Hydrology	2017	Canada	Identification of major nutrient sources and quantification of nutrient export from the catchment at different spatial scales.	total nitrogen, total phosphorous
Sediment load responses to climate variation and cascade reservoirs in the Yangtze River: A case study of the Jinsha River	Li; Lu; Yang; Chen; Lin	Geomorphology	2018	Singapore	The non-parametric Mann-Kendall test and double mass curve were used to explore the spatial-temporal variations of hydro-meteorological variables and quantify the contributions of climate variation and human activities to changes in discharge and sediment load in the JRB from the 1950s to 2015.	sediments
Impacts of Cascade Reservoirs on the Longitudinal Variability of Fine Sediment Characteristics: A Case Study of the Lancang and Nu Rivers	Guo; Zhu; Yang; Ma; Xiao; Ji; Liu	Journal of Hydrology	2020	China	Explores the impacts of cascade reservoirs on the grain size and mineral composition of fine sediments	sediments
Forecasting the remaining reservoir capacity in the Laurentian Great Lakes watershed	Alighalehbabakhani; Miller; Baskaran; Selegean; Barkach; Dahl; Abkenar	Journal of Hydrology	2017	USA	In this research, the sediment accumulation rates of twelve reservoirs within the Great Lakes watershed were evaluated using the Soil and Water Assessment Tool (SWAT). Based on the sediment accumulation rate, the remaining reservoir capacity for each study site was estimated.	sediments
A combined catchment-reservoir water quality model to guide catchment management for reservoir water quality control	Chen; Chong; Li	Water and Environment Journal	2021	China	The Hydrological Simulation Program-FORTRAN (HSPF) and the Water Quality Analysis Simulation Program (WASP), were adopted as a combined tool. This study demonstrated the usage of the combined model tool and the exceedance probability method in the data analysis, which could guide effective catchment management and eutrophication risk prevention.	total phosphorus

2.5 SUMMARY OF THE CHAPTER

The theoretical background provided an overview of studies developed in three different perspectives of the reservoirs planning and management. The first one (item 2.2) is the use of simplified models to facilitate the understanding of the waterbodies condition. This tendency of simplification can be complemented with the inclusion of the dynamic conditions that may affect the water quality. The second perspective (item 2.3) is the load orientated water quality analysis, which can be complimentary to the simplified modelling. The third facet (item 2.4) is the integration point of view of rivers and reservoirs modelling, which may be a promising outspread of the first and second perspectives.

The literature discussed in this research shows that the zero-dimensional, the integration of rivers and reservoirs and the TMDLs are potential tools to evaluate several water quality variables, as can be seen at Table 1 to Table 3. However, in this work the phosphorus was selected due to its importance justified at the introduction (item 1).

To sum up, the integration tools that consider loading inputs at rivers and reservoirs through simplified modelling still require more in-depth understanding and complementary computer tools that incorporate temporal dynamics.

3 MATERIAL AND METHODS

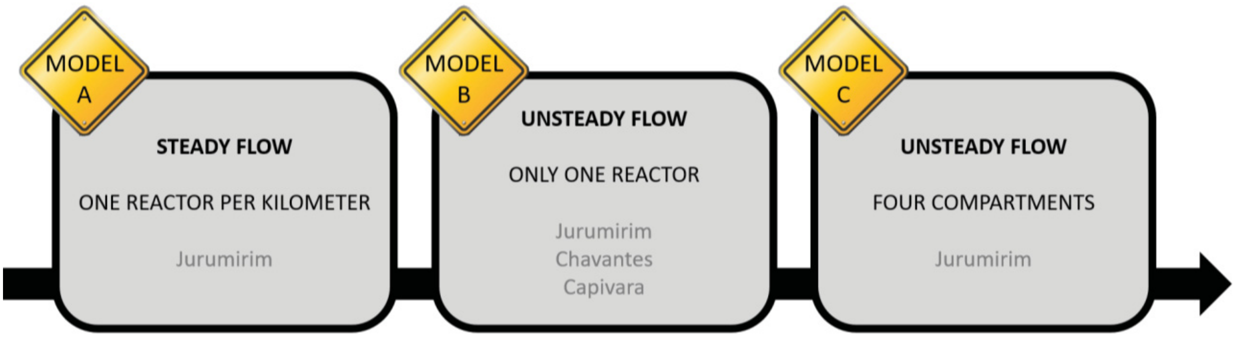
“Everything you can imagine is real.”
- Pablo Picasso

This item presents the research trajectory, the study area, the measured data sources and the equations applied to each model and other explanations necessary to results analysis.

3.1 RESEARCH TRAJECTORY

The research trajectory consisted in the development of three water quality models (Figure 3). The first one (model A), considered a steady flow and one reactor per kilometer in Jurumirim reservoir. Later, this model was left aside due to the possibility of adding the flow variations. Model B, which consisted on the unsteady flow CSTR model, was applied to Jurumirim, Chavantes and Capivara reservoirs. At last, in model C, the same unsteady flow CSTR model was applied to four different sectors of Jurumirim reservoir.

FIGURE 3 – RESEARCH TRAJECTORY FLUXOGRAM



3.2 STUDY AREA

The Paranapanema basin (Figure 4) is located in the States of São Paulo (47% of the basin) and Paraná (53%). The Paranapanema river rises in the Serra de Agudos Grandes, in São Paulo State, and has its mouth at Paraná River, after covering about 930 km. The headspring region is surrounded by intense native forest. Other data on vegetation cover and land use throughout the watershed can be consulted at ANA/UFPR (2019). The Paranapanema river was considered unsuitable for navigation due to the waterfalls along its course. From the 20th century onwards the energetic potential was discovered. Therefore, the greatest use today is power generation (IGIA, 2013). This research focused on the three biggest reservoirs of the Paranapanema River: Jurumirim, Chavantes and Capivara. Their main characteristics are described in Table 4.

FIGURE 4 – CASCADE RESERVOIRS ON PARANAPANEMA WATERSHED

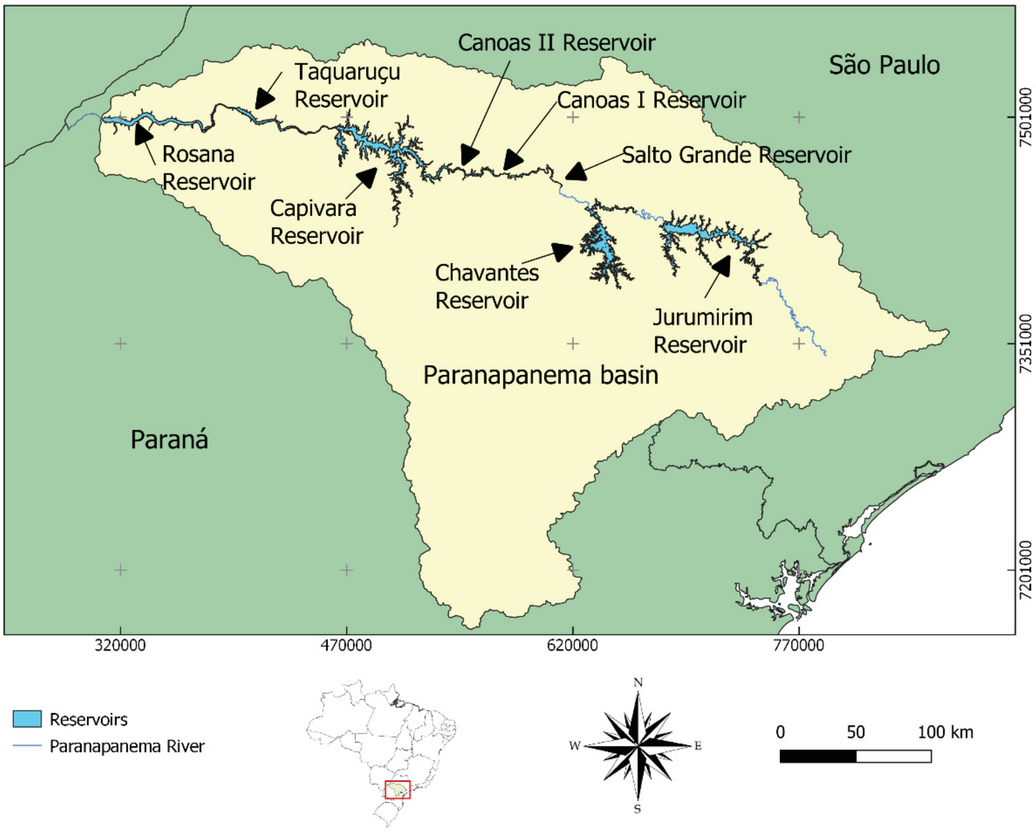


TABLE 4 – RESERVOIR'S CHARACTERISTICS

Power plant →	Jurumirim	Chavantes	Capivara
Inauguration year	1956	1959	1978
Power (MW)	98	414	619
Reservoir surface area (km^2) [a]	449	400	576
Residence Time (days) [a]	392	322	128
Average flow (m^3/s) [b]	263	394	1191
Volume ($10^6 m^3$) [a]	7107	8963	11623

(a) IGIA (2013);

(b) Considering the year 2012.

3.3 MEASURED DATA

This topic presents the sources of water quality data applied in the present study and their respective periods.

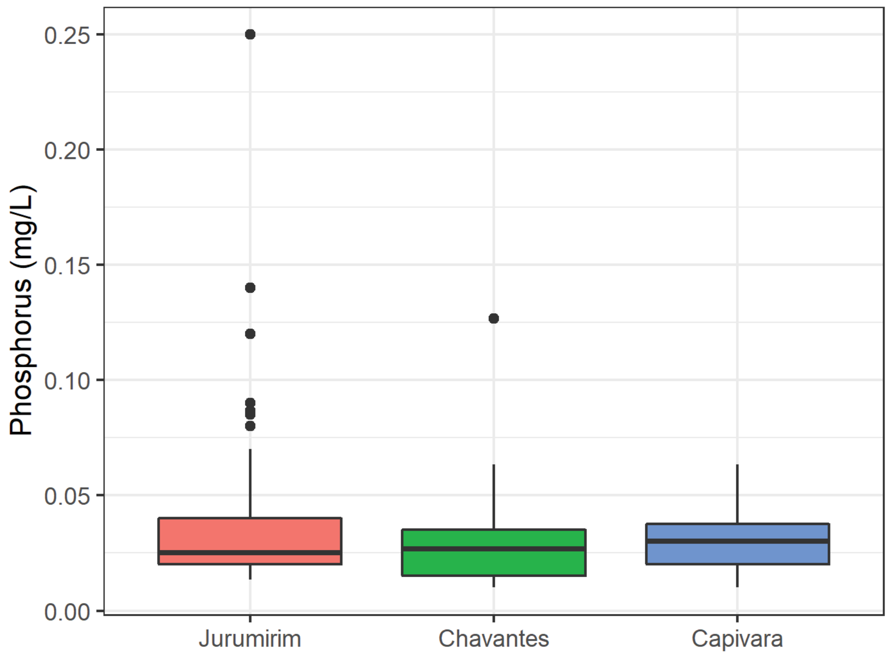
The Environmental Company of São Paulo State (CETESB) is responsible for the monitoring of water quality in São Paulo State. CETESB monitors the basin since January/1978 and the available data reaches until May/2018.

The HidroWeb Portal is a tool that is part of the National Water Resources Information System (SNIRH) and offers access to the database that contains all the information collected by the National Hydrometeorological Network (RHN), gathering data on river levels, flows, rainfall, climatology, water quality and sediments. The Paranapanema basin water quality data from this portal is available from August/1976 to April/2019.

IGIA (2013), indicated as “Envex” in the following figures and tables, developed a study of areas suitable for aquaculture in the Paranapanema Complex Reservoirs. This study generated water quality data from May/2011 to October/2011.

The datasets cited above did not presented constant frequencies. They were combined for each reservoir and can be summarized by boxplots in Figure 5.

FIGURE 5 – MEASURED DATA IN JURUMIRIM (N=84), CHAVANTES (N=22) AND CAPIVARA (N=32) RESERVOIRS



3.4 SYNTHETHIC SERIES

One peculiarity of the water quality monitoring is the scarce time scale, which is different from flow measurement time scales. Ferreira et al. (2019) applied an innovative method to match temporal scales of boundary conditions and generated synthetic pollutographs to convert a historical dataset (monitoring as snapshots during twelve years) into continuous information. The method allow this conversion by integrating the statistical parameters of the historical series and the natural random variability of the environment. The synthetic series generation was based on first order autoregressive process (AR1).

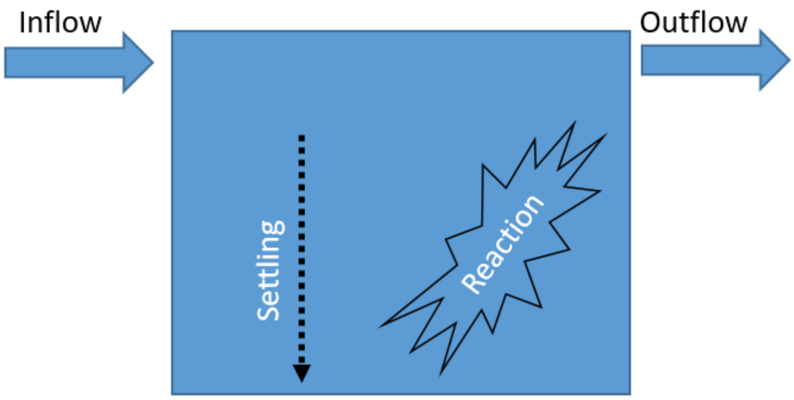
Due to the unavailability of water quality data in the same time scale of the hydrological data, ANA/UFPR (2020), based on the abovementioned study, calculated the synthetic series for the study case reservoirs and these results were applied in the present research, as well as in the three-dimensional model whose results were compared.

It is worth mentioning that exploring the challenges of time scales was not the goal of this research. However, this study present an important potential use to that authors' results.

3.5 CONTINUALLY STIRRED TANK REACTOR (CSTR)

The Continuously Stirred Tank Reactor (CSTR) is among the simplest ways to model a natural body of water (CHAPRA, 2008). The equations presented in this research indicate phosphorus concentrations. However, it is worth remembering that this methodology can be adapted to any water quality variable. This model considers the reaction and sedimentation processes represented in Figure 6 as described in Equation 1:

FIGURE 6 – NATURAL PROCESSES REPRESENTED IN CSTR MODEL



SOURCE: ADAPTATION FROM CHAPRA (2008)

$$Accumulation = inflow - outflow - reaction - settling \qquad (1)$$

Accumulation represents the change of mass in the system over time (t), as shown in Equation 2, in which V = volume (m³), c = phosphorus concentration (mg/L) and t = time (s).

$$Accumulation = \frac{dcV}{dt} \qquad (2)$$

The reaction is represented by the product of the first order reaction coefficient (k), volume (V) and concentration (c), as shown in Equation 3, in which k = first order decay coefficient (s^{-1}).

$$Reaction = k\,V\,c \qquad (3)$$

The settling is considered as the mass that goes through the water-sediment interface. Therefore, it's calculated by Equation 4, where v is the apparent settling velocity and H is the reservoir depth.

$$Settling = \frac{v}{H} V\, c \tag{4}$$

The equations of each process considered can by replaced in Equation 1, as shown in Equation 5, in which Q_{in}= inflow (m³/s), Q_{out} = outflow (m³/s), c_{in} = inlet concentrations (mg/L), c_{out} = outlet concentrations (mg/L) and A_s = surface area of the sediments (m²). The inflows and outflows are the multiplication of the inflow and outflow by the inlet and outlet concentrations, respectively.

$$\frac{dcV}{dt} = Q_{in}c_{in} - Q_{out}c_{out} - kVc - v\, A_s c \tag{5}$$

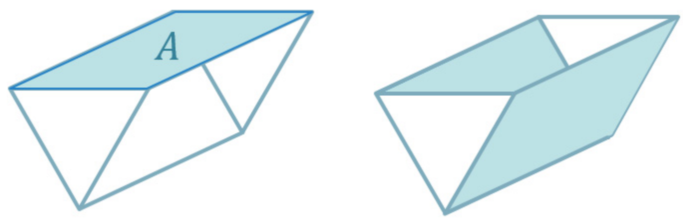
Using the numerical method of finite difference to approximate the derivative as differences, Equation 5 can be expressed as an algebraic Equation 6.

$$c_{out\, i+1} = \frac{c_{out\, i} + \frac{\Delta t}{V_{i+1}}\left(Q_{in\, i+1} c_{in\, i+1}\right)}{1 + \frac{\Delta t}{V_{i+1}}\left[Q_{out\, i+1} + kV_{i+1} + v\, A_{s\, i+1} + \frac{\Delta V}{\Delta t}\right]} \tag{6}$$

In which $c_{out\, i+1}$ = phosphorus concentration downstream (mg/L), $c_{out\, i}$ = phosphorus concentration downstream (when i=0, this value is equal to zero, since the initial condition applied in this research is that there was no phosphorus on the reservoir at first), $c_{in\, i+1}$ = phosphorus concentration upstream (mg/L), Δt = time step (s), V_{i+1}= volume of the corresponding reactor (m³), ΔV= difference of the volumes (m³), $Q_{in\, i+1}$ = Inflow (m³/s), $Q_{out\, i+1}$= Outflow (m³/s), k= first order decay coefficient (s^{-1}), v = apparent settling velocity (m/s) and $A_{s\, i+1}$= surface area of the sediments (m²).

The surface area of the sediment is estimated to be two times the surface area, supposing the reservoir has an equilateral triangle section (Figure 7).

FIGURE 7 – SIMPLIFICATION OF THE SURFACE AREA OF THE SEDIMENTS



3.6 MODEL A – RIVER-RESERVOIR INTEGRATED MODEL

The following model was developed in a previous phase of this dissertation project. However, throughout the time, the models B and C were prioritized over this one. Although model A is not taken into account for the zero-dimensional modelling purposes, it presents the idea of a river-reservoir integrated model, which can be explored in future studies.

The compartments in which this model was applied were different than the defined by the ANA/UFPR project group in ANA/UFPR (2021), since it was done prior to the final definition.

Also, the equation of the model is different from the one presented in item 3.5, which is valid for the models B and C. While in this model the equation for constant volume is presented by Chapra (2008), the models B and C use the equation derived in APPENDIX A, considering variable volume.

a) <u>Preliminary definition of compartments</u>

Aiming to consider the different characteristics of the studied reservoir along its length, it was separated in three compartments: C1, C2 and C3 (Figure 8). The variables depth, velocity and volume were considered as medium values for each compartment. In the reservoir compartments (from km 30 to km 147), the model was applied for each kilometer (Δx), considering Table 5. In the river reaches, a first order decay model was applied.

FIGURE 8 – JURUMIRIM COMPARTMENTS

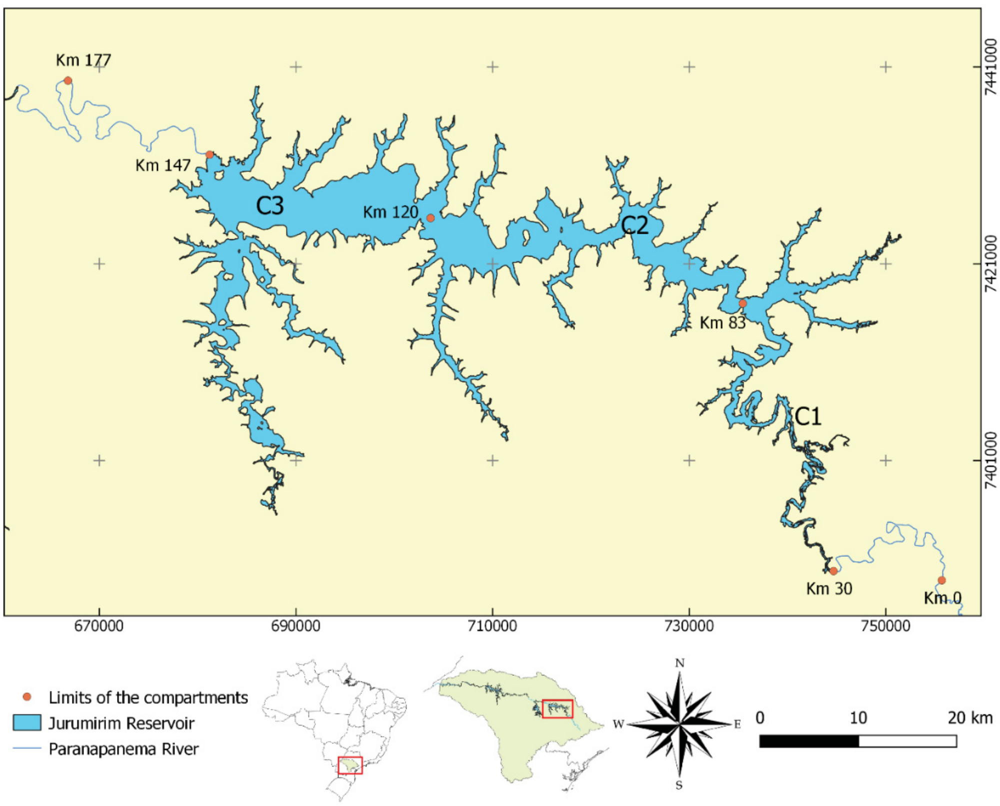


TABLE 5 – DATA APPLIED TO THE SIMULATION

Reach	River (Upstream)	Reservoir (C1)	Reservoir (C2)	Reservoir (C3)	River (Downstream)
Model	Simplified first order decay model	CSTR	CSTR	CSTR	Simplified first order decay model
Distance (km)	0 to 30	30 to 83	83 to 120	120 to 147	147 to 177
Medium Depth (m)	-	6.77	12.74	12.41	-
Estimated volume for the reach (10^6 m³)	-	136.94	56.88	16.85	-
Estimated volume per kilometer for the reach (10^6 m³/km)	-	2.58	1.54	0.62	-
Velocity (m/s)	0.750	0.0127	0.0058	0.0011	0.750
k (day^{-1})	0.80	0.101	0.101	0.101	0.80

The apparent settling velocity (v) was constant along the reservoir reaches (1 10^{-4} m/day). The model was applied considering a steady situation, with flow of 107 m³/s, which is the 95 quantile of the 2012 flows, and volume of 210.67 10^6 m^3.

The reservoir velocities were estimated so that the time water spends inside the reactor is equal to the residence time (391.72 days).

b) <u>Water Quality Stations</u>

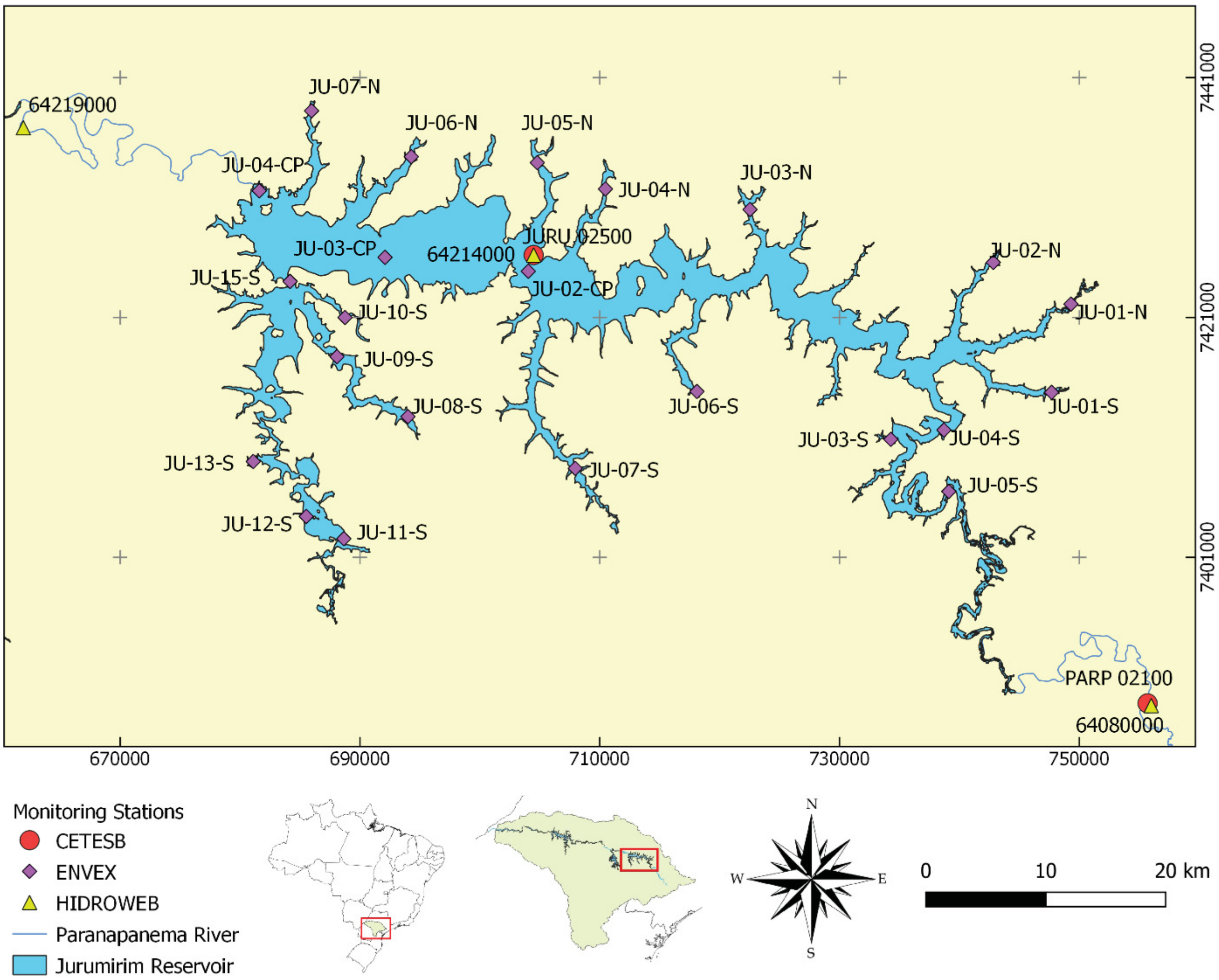
The water quality stations of Jurumirim reservoir are shown in Table 6, from upstream to downstream. The column kilometer indicates the distance from the first station of the river (PARP 02100, which is coincident to 64080000). Water quality stations with the same coordinates are coincident points. The reservoir starts at 30 km and ends at 147 km. Table 9 illustrates the location of the monitoring stations. Despite of the stations location was geographically distributed, each ENVEX station was monitored for a short period of time (march/2011 to april/2011). In Jurumirim reservoir, for example, this monitoring resulted in 24 values of total phosphorus distributed along the reservoir. Those results were consolidated with more 60 results of total phosphorus obtained in Hidroweb (February/2001 to December/2010). Only the water surface data was selected for analysis.

TABLE 6 – JURUMIRIM WATER QUALITY STATIONS

Station	Location	Kilometer	Source	Latitude	Longitude
PARP 02100	River	0	CETESB	755.698	7.388.804
64080000	River	0	HIDROWEB	756.005	7.388.611
JU-02-S	Reservoir Center	58	ENVEX	739.119	7.406.482
JU-05-S	Reservoir Center	58	ENVEX	739.119	7.406.482
JU-03-S	Reservoir Center	70	ENVEX	734.281	7.410.827
JU-04-S	Reservoir Center	74	ENVEX	738.707	7.411.601
JU-01-N	Reservoir Arm	80	ENVEX	749.310	7.422.106
JU-01-S	Reservoir Arm	80	ENVEX	747.693	7.414.752
JU-02-N	Reservoir Arm	80	ENVEX	742.830	7.425.580
JU-03-N	Reservoir Arm	97	ENVEX	722.532	7.429.991
JU-06-S	Reservoir Arm	103	ENVEX	718.102	7.414.820
JU-04-N	Reservoir Arm	115	ENVEX	710.471	7.431.709
JU-07-S	Reservoir Arm	115	ENVEX	707.951	7.408.402

Station	Location	Kilometer	Source	Latitude	Longitude
JU-02-CP	Reservoir Center	119	ENVEX	704.035	7.424.846
JURU 02500	Reservoir Center	120	CETESB	704.483	7.426.200
64214000	Reservoir Center	120	HIDROWEB	704.482	7.426.197
JU-05-N	Reservoir Arm	121	ENVEX	704.785	7.433.903
JU-03-CP	Reservoir Center	132	ENVEX	692.082	7.426.005
JU-06-N	Reservoir Arm	138	ENVEX	694.272	7.434.402
JU-08-S	Reservoir Arm	142	ENVEX	693.996	7.412.724
JU-09-S	Reservoir Arm	142	ENVEX	688.070	7.417.721
JU-10-S	Reservoir Arm	142	ENVEX	688.743	7.420.988
JU-11-S	Reservoir Arm	142	ENVEX	688.647	7.402.538
JU-12-S	Reservoir Arm	142	ENVEX	685.513	7.404.390
JU-13-S	Reservoir Arm	142	ENVEX	681.088	7.408.977
JU-15-S	Reservoir Arm	142	ENVEX	684.163	7.423.999
JU-LE	Reservoir Arm	142	ENVEX	684.163	7.423.999
JU-07-N	Reservoir Arm	144	ENVEX	685.957	7.438.228
JU-04-CP	Reservoir Center	146	ENVEX	681.594	7.431.554
64219000	River	175	HIDROWEB	661.912	7.436.813

FIGURE 9 – JURUMIRIM MONITORING STATIONS



c) <u>River compartments</u>

In the river compartments, a simplified first order decay model was applied (Equation 7). In which C_i= phosphorus concentration (mg/L), C_{i+1}= phosphorus concentration in the next time step (mg/L), k= first order decay coefficient (s^{-1}) and Δt= time step (s).

$$C_{i+1} = C_i \times e^{-k\frac{\Delta x}{U}} \tag{7}$$

d) <u>Reservoir compartments</u>

Equation 8 (CHAPRA, 2008) is applied on the reservoir compartments. The λ is given by Equation 9, in which c_0 = initial phosphorus concentration (mg/L) and λ = constant (s^{-1}).

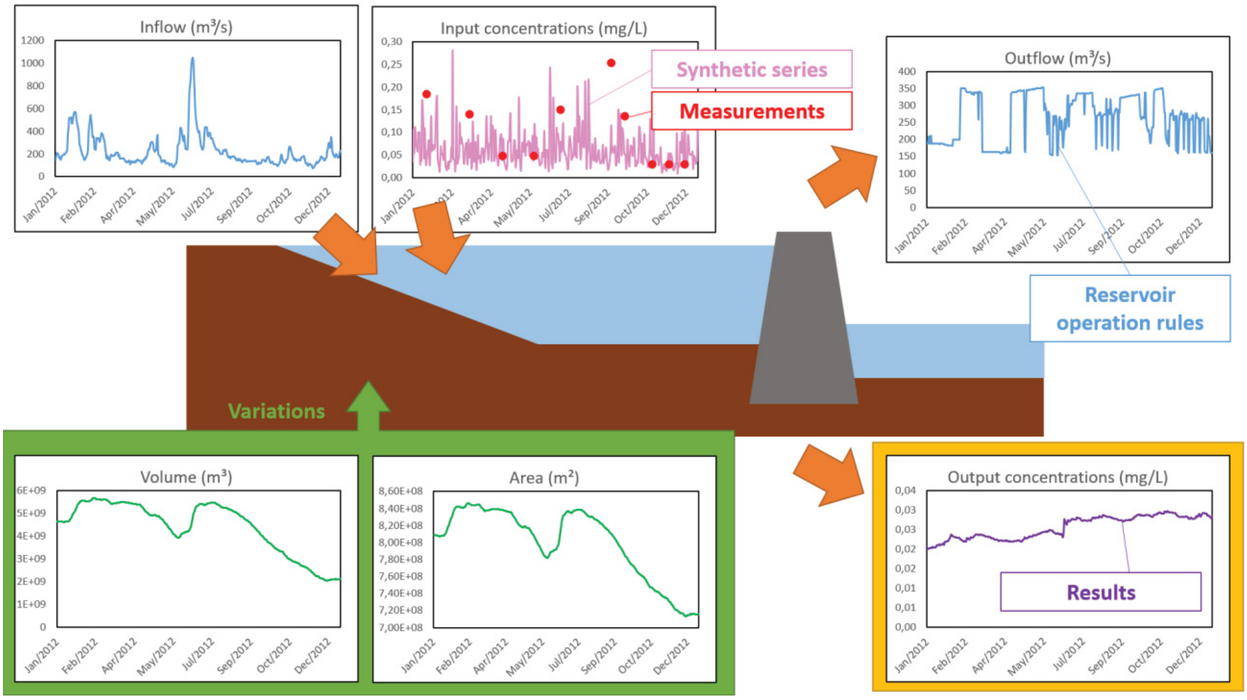
$$c = c_0 e^{-\lambda t} + \frac{W}{\lambda V}\left(1 - e^{-\lambda t}\right) \tag{8}$$

$$\lambda = \frac{Q}{V} + k + \frac{v}{H} \tag{9}$$

3.7 MODEL B – CONTINUALLY STIRRED TANK REACTOR (CSTR): A ZERO-DIMENSIONAL MODEL

This model was based on the unsteady CSTR model presented in item 3.5. It was run for a period of two years. The first-year results were discarded in order to guarantee that the warm up time had no influence on the results. For each day, there was a value of inflow, outflow, volume, area and input concentration. The flows, areas and volumes came from the Brazilian reservoir tracking system (SAR). The daily input concentrations are the results from the synthetic series of ANA/UFPR (2020). Figure 10 shows a schematic illustration of the input and output data of the model.

FIGURE 10 – SCHEMATIC ILLUSTRATION OF THE INPUT AND OUTPUT DATA OF THE MODEL



The parameters k and v were chosen based on the comparison of the boxplots to the observed data. This comparison is presented in the item 4.3.

The simulations were made for a base scenario and four future scenarios: B12, T25, T35, A25 and A35, as described in Table 7. Those scenarios were defined by ANA/UFPR (2020), based in economic scenarios shown in Integrated Water Resources Plan of the Paranapanema Water Resources Management Unit (ANA/CBH PARANAPANEMA, 2016). In the tendential scenarios, public policies and the cultural socioeconomic arrangement will not differ radically from current ones. Brazil's short-term trend scenario brings stagnation to this basin until 2020, a moderate increasing in the economy until 2025 and a large increase until 2035. The accelerated scenarios represent the hypothesis of a series of positive factors joined, creating favorable conditions to economic growth. In this scenario, the wide increase in the economy starts from the year 2025 and it is maintained until 2035.

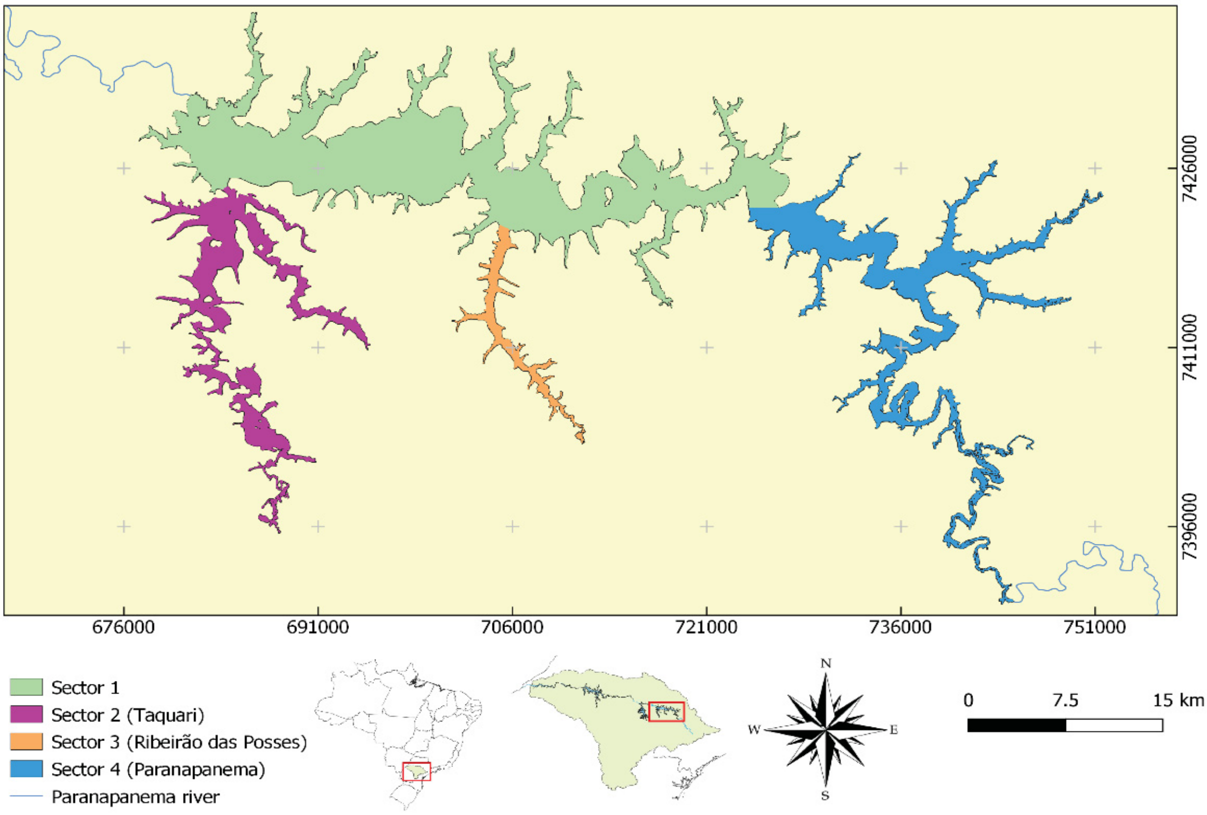
TABLE 7 – FUTURE SCENARIOS

B12	Baseline scenario - 2012	The year 2012 was selected for the reference scenario due to the availability of flow and concentration data.
T25	Tendential scenario - 2025	Brazil's short-term trend economic scenario for the year 2025, considering a moderate increment in the economic situation.
T35	Tendential scenario - 2035	Brazil's long-term trend economic scenario for the year 2035, considering a moderate increment in the economic situation.
A25	Accelerated scenario - 2025	Brazil's short-term trend economic scenario for the year 2025, considering a wide increment in the economic situation.
A35	Accelerated scenario - 2035	Brazil's long-term trend economic scenario for the year 2035, considering a wide increment in the economic situation.

3.8 MODEL C – CSTR MODEL WITH COMPARTMENTS

The CSTR model explained in item 3.5 is also applied in the four sectors of the Jurumirim reservoir (Figure 11) defined by ANA/UFPR (2021), aiming to create zones with similar water quality characteristics. The number of sectors were defined as the total number of the largest sub-basins covering 80% of total reservoir’s drainage area. The definition of sector was the result of spectral clustering of equidistant points inside the reservoir area. Thus, the result is a clustering based on the morphological aspects of the reservoir and the basin.

FIGURE 11 – SECTORS APPLIED IN "MODEL C"



The outlet flows and concentrations of the sectors 2, 3 and 4 were considered as input values for the sector 1, as showed by Equation 10. This equation is the same as Equation 6, but the terms Q_{in} and c_{in} for each sector were included.

$$\overbrace{c_{out\,i+1}}^{\text{Sector 1}} = \frac{c_{out\,i} + \frac{\Delta t}{V_{i+1}}\left(\overbrace{Q_{in\,i+1}c_{in\,i+1}}^{\text{Sector 1}} + \overbrace{Q_{out\,i+1}c_{out\,i+1}}^{\text{Sector 2}} + \overbrace{Q_{out\,i+1}c_{out\,i+1}}^{\text{Sector 3}} + \overbrace{Q_{out\,i+1}c_{out\,i+1}}^{\text{Sector 4}}\right)}{1 + \frac{\Delta t}{V_{i+1}}\left[Q_{out\,i+1} + kV_{i+1} + v\,A_{s\,i+1} + \frac{\Delta V}{\Delta t}\right]} \tag{10}$$

Due to the lack of sufficient observed data for comparison of the results of each sector, the choice of the parameters k and v followed the same values applied for model B for the Jurumirim reservoir. The parameters were the same for all the sectors.

3.9 THREE-DIMENSIONAL MODEL: DELFT3D

The three-dimensional modeling considered in the comparison with the zero-dimensional model was conducted by ANA/UFPR (2020) on Delft3D mathematical model. In the horizontal direction, 98.646 cells were defined (401 in x direction in the Cartesian plan, 246 in y direction in the Cartesian plan). Figure 12 illustrates the morphologic grid. In the vertical direction, 10 layers were considered. The time step of the simulation was 30 seconds, in order to assure the Courant criteria and the stability of the numerical solution. In this case, the initial level was -2 m and the initial temperature was 20ºC. The phosphorus concentration series considered in the comparison were the vertical depth averaged results simulated in the exit of each sector. Figure 13 presents the output monitoring points in which the daily series were evaluated. The values selected for the analysis were the average concentrations of the water column.

FIGURE 12 – MORPHOLOGIC GRID FOR JURUMIRIM RESERVOIR

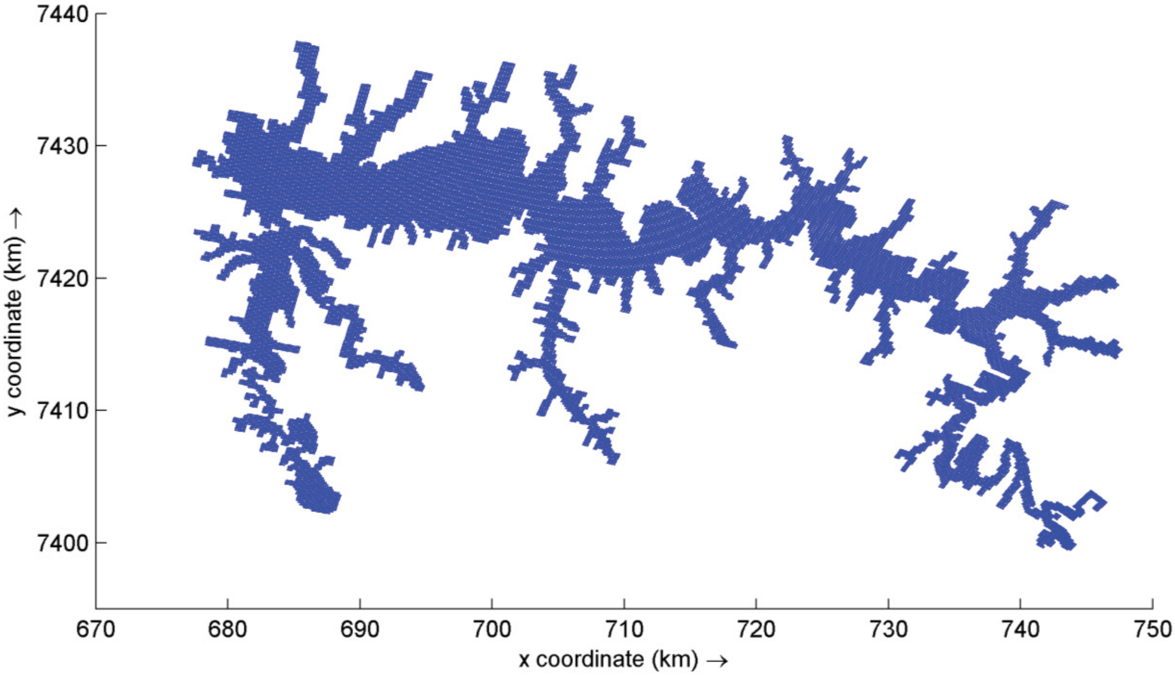
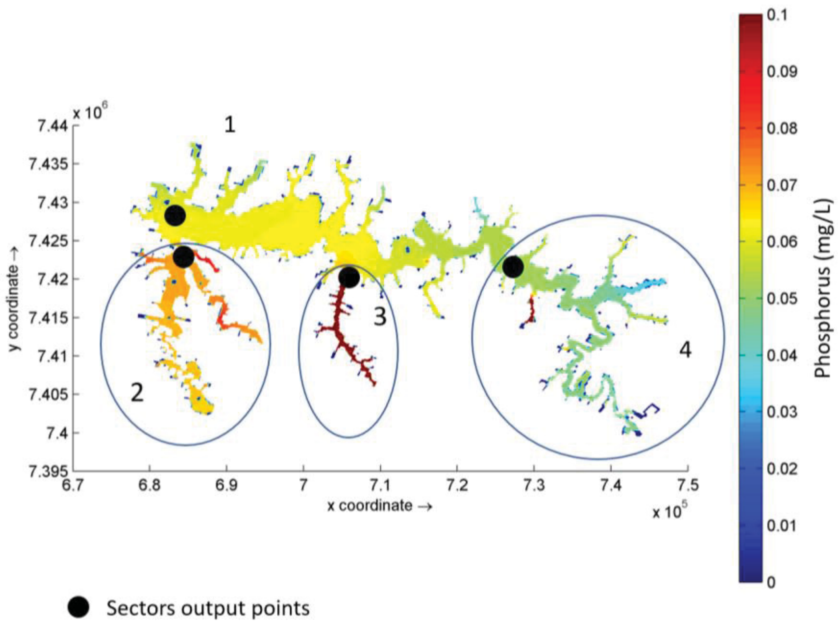


FIGURE 13 – MONITORING WATER QUALITY DATA FROM DELFT3D MODEL USED FOR COMPARISON BETWEEN MODELS



3.10 TOTAL MAXIMUM DAILY LOAD (TMDL)

The Total Maximum Daily Loads are the maximum amount of a pollutant allowed to enter a waterbody so that it will still respect the water quality standards for that particular pollutant. A possible way to estimate the acceptable load (pollutant cap) is calculating the corresponding load compatible with the water quality standards. Therefore, the TMDLs were calculated based on the daily flows of the reference year (2012) and the phosphorus concentration limits for lentic environments from CONAMA 357/2005 resolution.

The first step was to integrate the limit daily loads through the year and get to the Total Maximum Annual Load (TMAL), in ton/year, according to Equation 11, in which i represents the day of the year, Q_i is the flow registered in the respective day (m³/s), CL is the concentration limit from CONAMA 357/2005 resolution (mg/L) and 86,4 is a factor for transformation of units.

$$TMAL = \sum_{i=1}^{366} \frac{Q_i \times CL}{86{,}4} \tag{11}$$

The TMAL divided by the 366 days of the year represents the TMDL (ton/day), according to Equation 12.

$$TMDL = \frac{TMAL}{366} = \sum \frac{Q_i \times CL}{31622{,}4} \tag{12}$$

3.11 DATA ANALYSIS: TROPHIC STATE INDEX (TSI) AND BRAZILIAN RESOLUTION

In order to show the magnitude of the phosphorus values, they were compared to the Trophic State Index (TSI) and also to the limits of the Brazilian resolution CONAMA 357/2005.

- Trophic State Index (TSI)

Eutrophication takes place in lentic environments and occurs by increasing the concentrations of nutrients, such as phosphorus and nitrogen. This causes the occurrence of phytoplankton and aquatic macrophytes to increase. According to Esteves (1998), phosphorus is the main responsible for the eutrophication of ecosystems and acts as a limiting factor of productivity in most continental waters. The TSI makes it possible to assess the effects of nutrient enrichment on water quality. The index classifies the water body in degrees of trophy, according to Table 8.

TABLE 8 – TROPHIC STATE INDEX AND DEGREES OF TROPHY

Category	Result of TSI
Ultraoligotrophic	TSI ≤ 47
Oligotrophic	47 < TSI ≤ 52
Mesotrophic	52 < TSI ≤ 59
Eutrophic	59 < TSI ≤ 63
Supereutrophic	63 < TSI ≤ 67
Hypereutrophic	TSI > 67

SOURCE: LAMPARELLI (2004)

Lamparelli (2004) proposes the following equations for the TSI calculation, where P is the total phosphorus concentration, in µg/L.

$$\mathrm{TSI}_{\mathrm{River}} = 10 \times \left[6 - \left(\frac{0.42 - 0.36 \ln P}{\ln 2}\right)\right] - 20 \tag{13}$$

$$\mathrm{TSI}_{\mathrm{Reservoir}} = 10 \times \left[6 - \left(\frac{1.77 - 0.42 \ln P}{\ln 2}\right)\right] \tag{14}$$

- Brazilian resolution

The Brazilian Water Quality Classification Framework system states that water uses are conditioned by its quality. Higher quality waters allow more demanding uses, while lower quality waters allow only less demanding uses. The classification system is illustrated by Figure 14, where the water uses indicated by the resolution match to the colored rectangles for each class.

FIGURE 14 – WATER QUALITY CLASSIFICATION FRAMEWORK OF WATERBODIES

FRESHWATER USES	SPECIAL	1	2	3	4
Preserving the natural balance of aquatic communities	Mandatory class in conservation units				
Protection of aquatic communities		Mandatory class in indigenous lands			
Primary contact recreation					
Aquaculture					
Supply for human consumption	After disinfection	After simplified treatment	After conventional treatment	After conventional or advanced treatment	
Secondary contact recreation					
Fishing					
Irrigation		Vegetables eaten raw and fruits that thrive close to the ground and eaten raw without peeling	Vegetables, fruits, parks, gardens, sports and leisure fields	Tree, cereal and forage crops	
Animal watering					
Navigation					
Landscape harmony					

SOURCE: ADAPTED FROM ANA (2021)

The measured and simulated data was also compared to the Class 2 limits of the CONAMA 357/2005 resolution (BRASIL, 2005). For lotic environment (rivers and streams) the limit is 0.1 mg/L, while for lentic environments (lakes and reservoirs) the limit is equal to 0.03 mg/L. The Class 2 limits were applied as reference values aiming better understanding of phosphorus values due to the article 42 of the aforementioned resolution, which indicates that while the Water Quality Classification Framework is not approved, freshwater is considered as Class 2. The phosphorus limits for class 1 (0.02 mg/L) and class 3 (0.05 mg/L) in lentic environments were also applied in results discussion.

4 RESULTS AND DISCUSSION

"People who wonder if the glass is half empty or full miss the point. The glass is refillable."
- Unknown

In this item, Total Maximum Daily Loads results are presented, as well as the phosphorus concentrations and loads simulated by zero-dimensional models. Ultimately, the comparison of those results with a 3D model is showed in item 4.5.

4.1 TOTAL MAXIMUM DAILY LOADS (TMDL)

Considering the daily time series of inflows and outflows for the year 2012, the limit loads were calculated for each day, according to the procedure expressed in item 3.10. This calculation was made by multiplying the daily flow per the limit concentration of each water quality class of CONAMA 357/2005 resolution. The sum of this daily values represents the TMAL and the mean represents the TMDL. The TMALs and the TMDLs are shown in Table 9, as well as the phosphorus concentration limits for lentic environments.

TABLE 9 – PHOSPHORUS LIMITS, TMAL AND TMDL

Phosphorus limits (mg/L)			TMAL (ton/year)			TMDL (ton/day)		
			Jurumirim	Chavantes	Capivara	Jurumirim	Chavantes	Capivara
Inflow	Class 1	0.02	291 727	441 102	291 727	399	603	399
	Class 2	0.03	437 591	661 653	437 591	599	905	599
	Class 3	0.05	583 454	882 205	583 454	798	1207	798
Outflow	Class 1	0.02	306 967	453 768	1 499 208	420	621	2 051
	Class 2	0.03	460 451	680 651	2 248 811	630	931	3 076
	Class 3	0.05	613 934	907 535	2 998 415	840	1241	4 102

Therefore, Table 9 answers the question: "How much pollution is the reservoir capable of receive without compromising the reservoir planning and management?" for each one of the Water Quality Framework class.

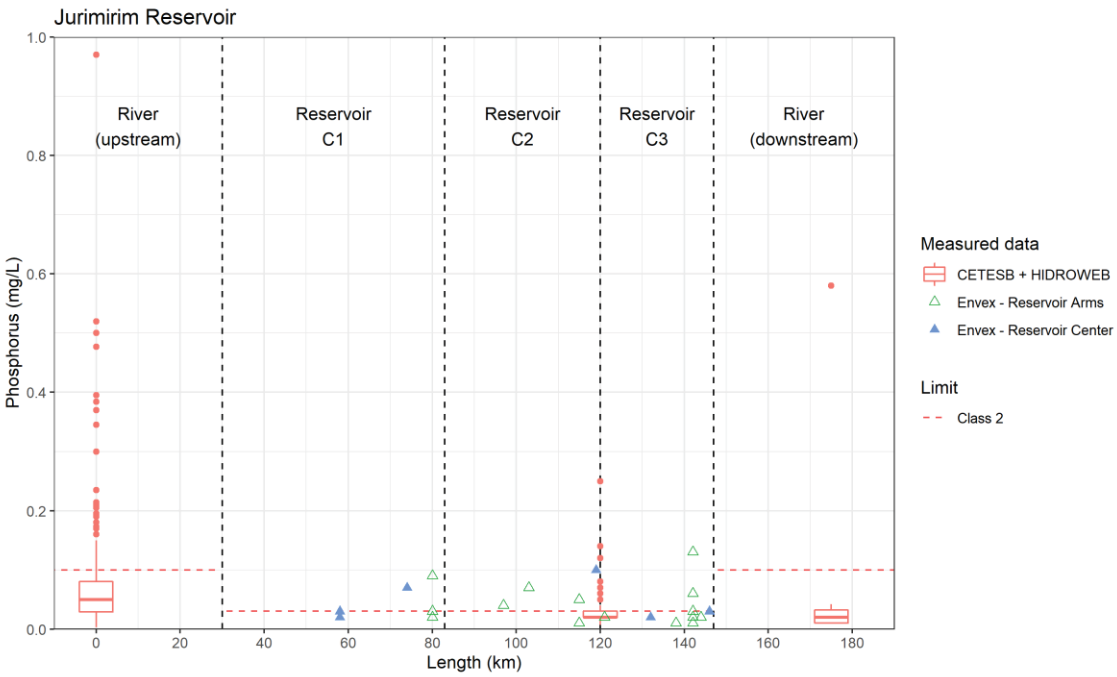
4.2 MODEL A – STEADY FLOW STATE

The first model was the River-Reservoir Integrated Model for Steady Flow State. Models B and C were prioritized over this one, due to the capability of including the flow variations in unsteady state models. Although model A is not taken into account for the zero-dimensional modelling purposes, it presents the idea of a river-reservoir integrated model, which can be explored in future studies.

Three different phosphorus fractions were measured along the monitoring period. Due to the scarcity of data, the bigger fraction available on the dataset for each station and date was considered as total phosphorus for modeling purposes. It was accepted that it might underestimate the phosphorus concentrations.

In the Paranapanema river, upstream of the Jurumirim reservoir, 15% of 290 the concentrations were above the Class 2 limit (0.1 mg/L). In the reservoir, where the limit is 0.03 mg/L, 24% of the 189 observed concentrations exceeded the limit. Downstream, one of the twelve measured concentrations exceeded the lotic limit, which represents 8% of exceedance. The measured data was compared, in Figure 15, to the Class 2 limits of the CONAMA 357/2005 resolution (BRASIL, 2005).

FIGURE 15 – OBSERVED PHOSPHORUS DATA IN JURUMIRIM RESERVOIR



The River-Reservoir Integrated Model (RRIM) was applied as explained in item 3.6. Figure 16 shows the observed data for Jurumirim reservoir and the river upstream, as well as the results for the River-Reservoir Integrated Model (RRIM).

In the first scenario (RRIM_1), the initial values defined for the river and the reservoir were defined as the mean from the observed data in each environment. In the second scenario (RRIM_2), the initial values were defined as the 99 quantile of the observed series.

In this simulation, no loads were added in the model besides the initial values concentrations. The vertical dashed lines represent the limits of the reservoir compartments.

FIGURE 16 – RIVER-RESERVOIR INTEGRATED MODEL AND OBSERVED DATA IN JURUMIRIM RESERVOIR

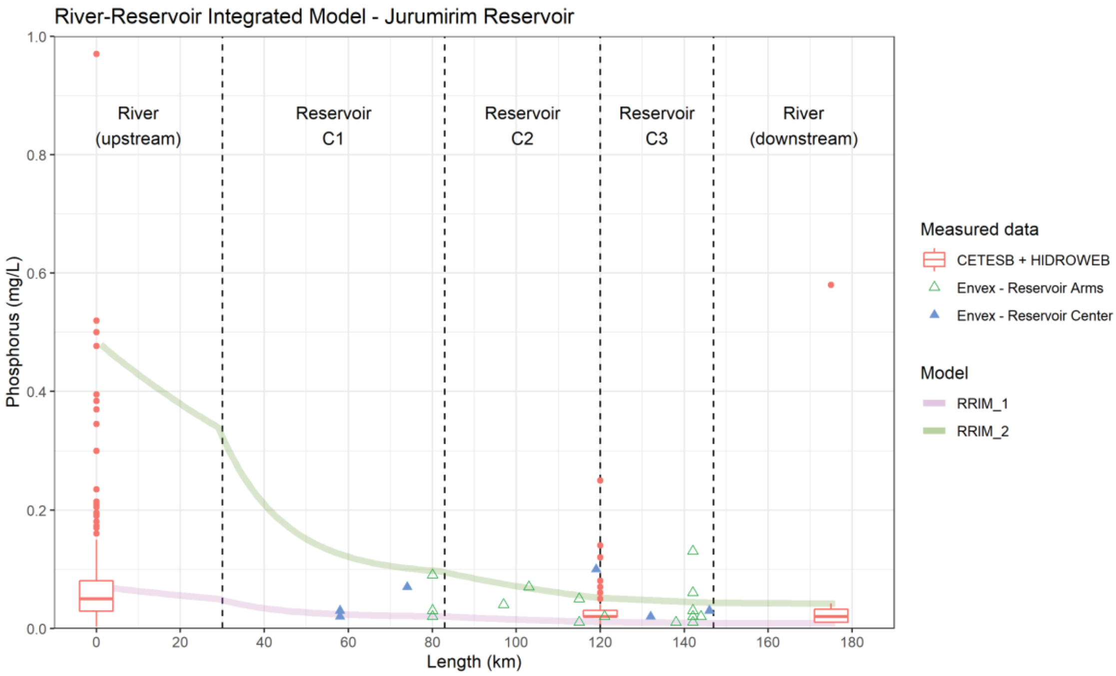


Figure 17 shows the same simulation, as function of time. Due to the high velocities in the river reaches and, consequently, the quick decrease of the concentration, they do not appear in the figure. Figure 18 shows the estimated velocities in the three reservoir compartments. The velocities were defined so that the residence time of the reservoir is the same found in literature. They are also described in Table 5.

FIGURE 17 – RIVER-RESERVOIR INTEGRATED MODEL AS FUNCTION OF TIME IN JURUMIRIM RESERVOIR

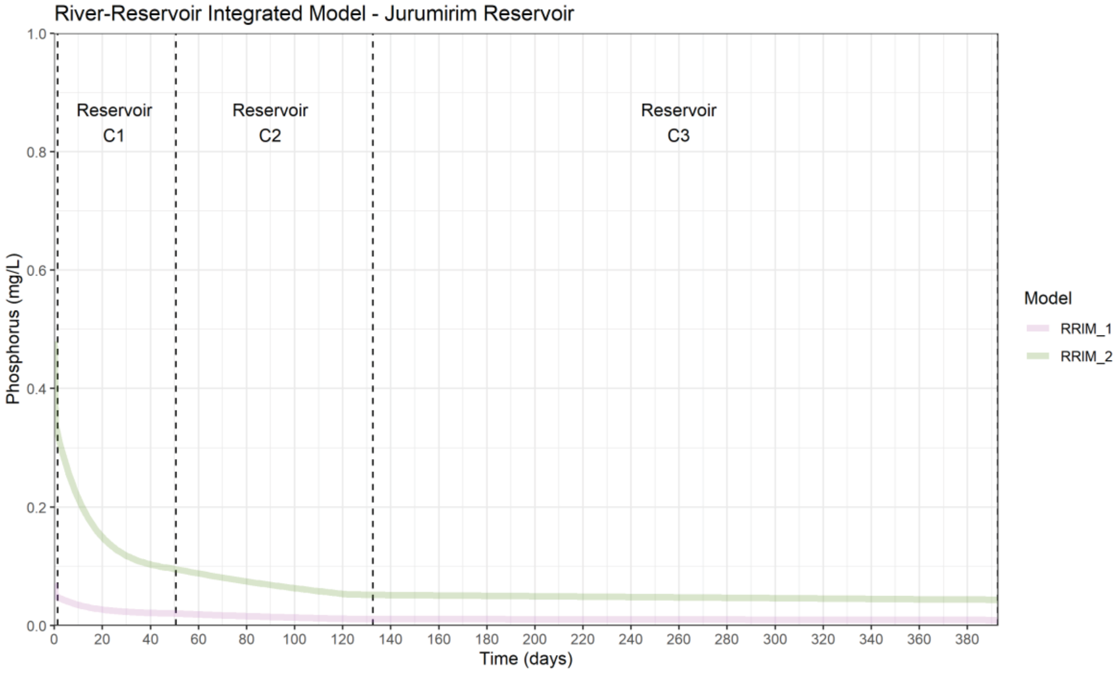


FIGURE 18 – VELOCITIES IN JURUMIRIM RESERVOIR

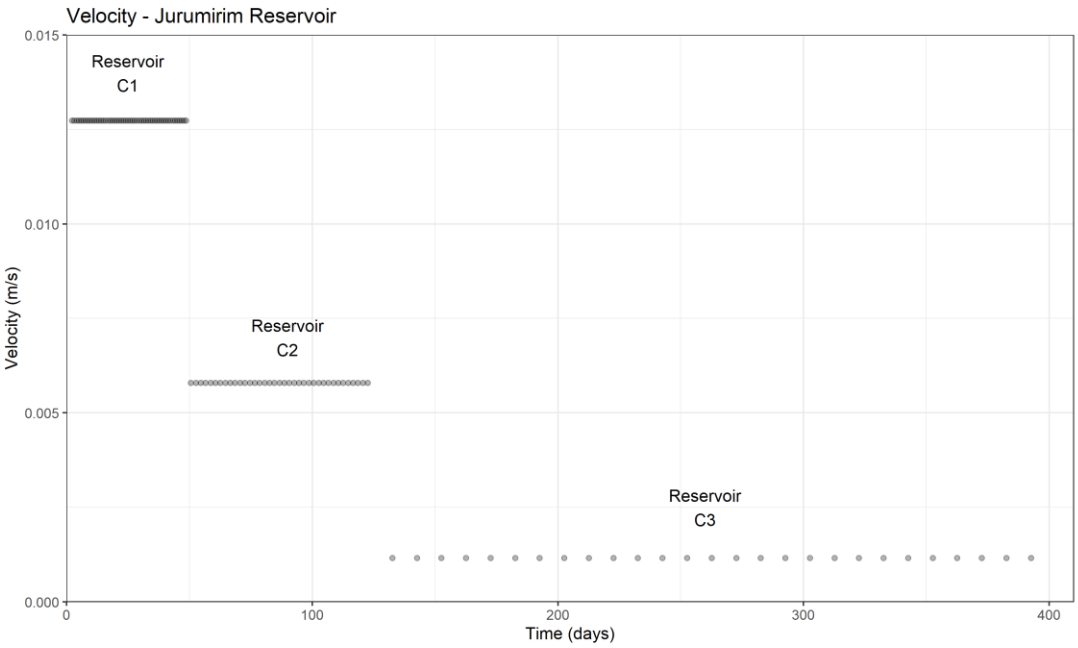


Figure 19 presents the Trophic State Index for the simulated and observed values. For the RRIM_1 simulation, the TSI resulted as Mesothophic in 51% of the length of the reservoir, and in the rest of the length, it was divided between Oligrotrophic (33%) and Ultraoligotrophic (17%).

For the RRIM_2 simulation, the TSI resulted as Mesothophic in 36% of the length of the reservoir, and in the rest of the length, it was divided between Eutrophic (28%), Supereutrophic (32%) and Hypereutrophic (5%).

The observed data, however, results mostly in the classes Mesothophic (61%) and Oligotrophic (20%), which shows that the RRIM_1 simulation is more similar to the observed values. This results were expected since RRIM_2 applied the observed data 99 quantile as initial value.

FIGURE 19 – TROPHIC STATE INDEX FOR THE OBSERVED AND SIMULATED VALUES

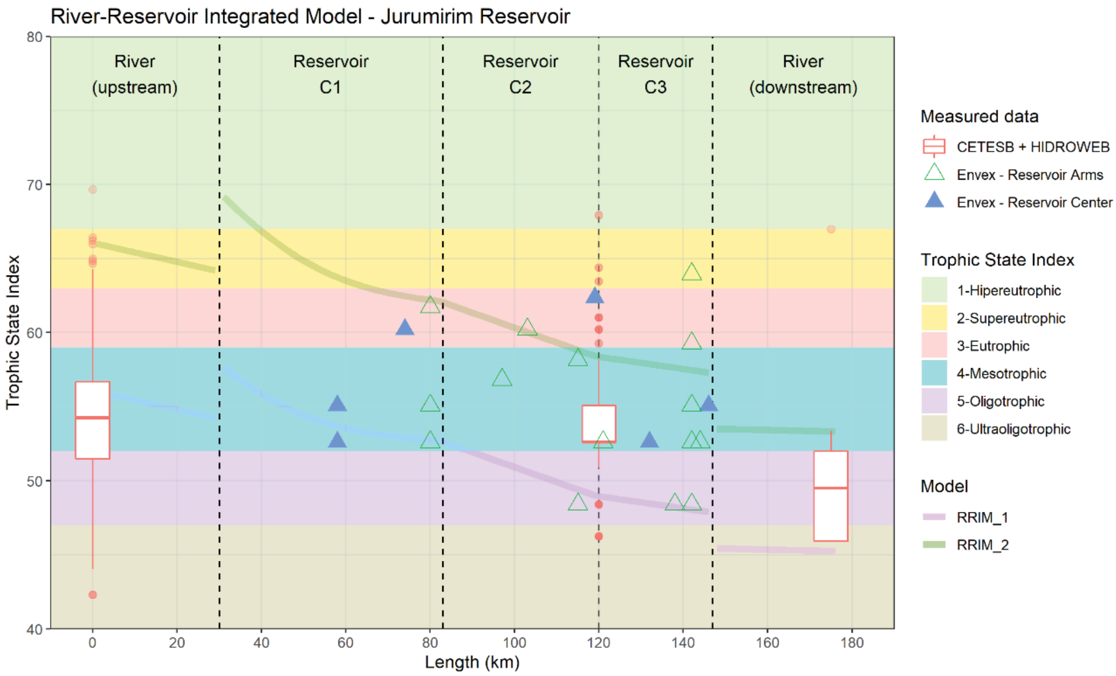


Figure 20 and Figure 21 show the tests of different reaction coefficients (k) for RRIM_1 and RRIM_2, respectively. They vary from 0.01 day^{-1} to 0.10 day^{-1}. The model results respond well to the k variation, with smaller concentrations as the k value grows.

FIGURE 20 – DIFERRENT REACTION COEFFICIENTS FOR RRIM_1

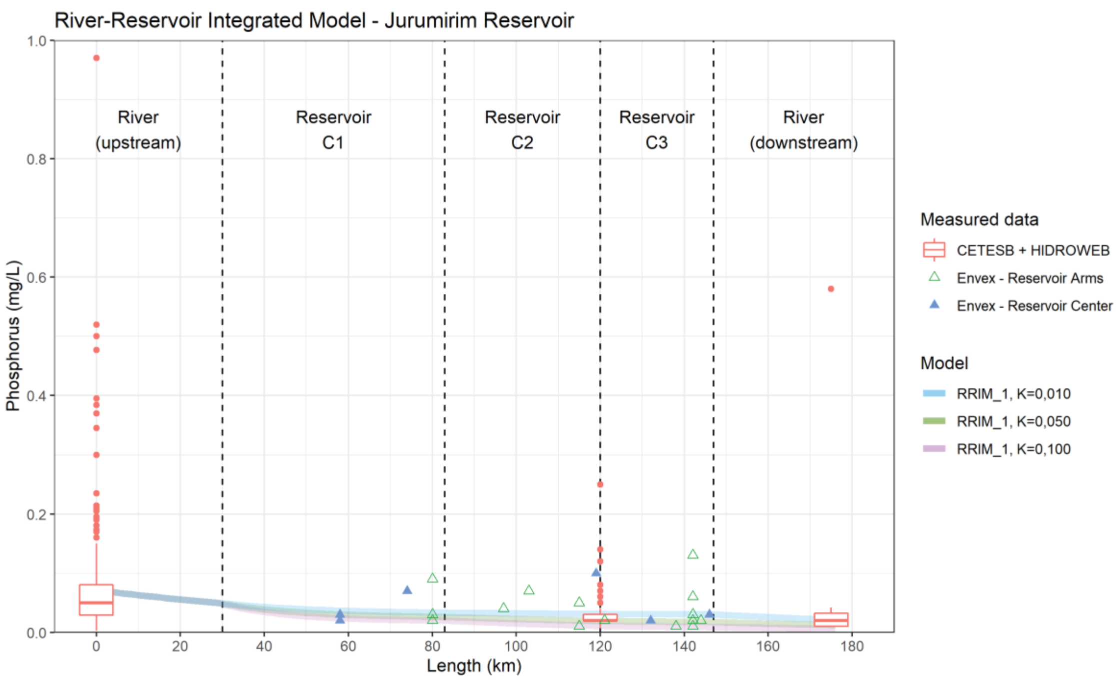
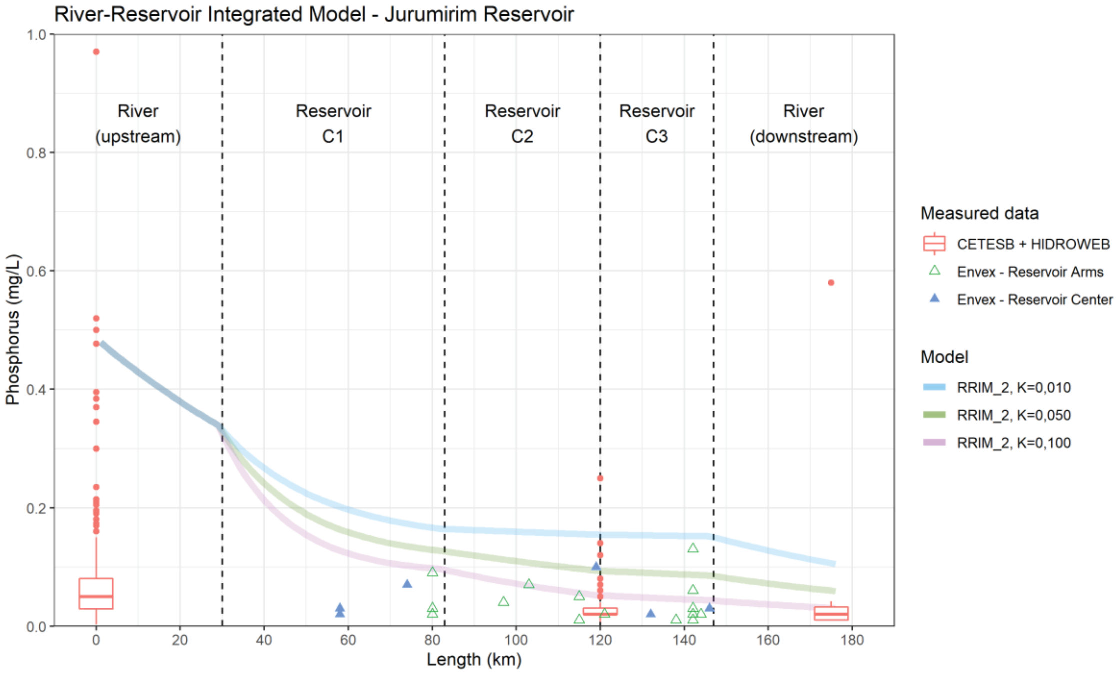


FIGURE 21 – DIFERRENT REACTION COEFFICIENTS FOR RRIM_2



4.3 MODEL B – UNSTEADY FLOW STATE

This model was based on the unsteady CSTR model presented in topics 3.5 and 3.7. The calibration of the model consisted in the process of comparing the boxplots of several simulated series with the boxplot of the measured data. The simulated series were calculated considering the first order decay coefficient (k) of 0 s^{-1}, 0.001 s^{-1}, 0.005 s^{-1} and 0.010 s^{-1}. The apparent settling velocity (v) values were 0 m/s, 0.001 m/s and 0.010 m/s.

Figure 22 shows the water quality calibration boxplots for Jurumirim reservoir. In the right, the last boxplot shows the observed data for water quality stations of Jurumirim reservoir. The blue horizontal line is the median of observed data.

FIGURE 22 – BOXPLOTS OF THE SENSIBILITY ANALISYS OF THE MODEL PARAMETERS: JURUMIRIM RESERVOIR (THE BLUE LINE REPRESENTS THE MEDIAN OF OBSERVED DATA)

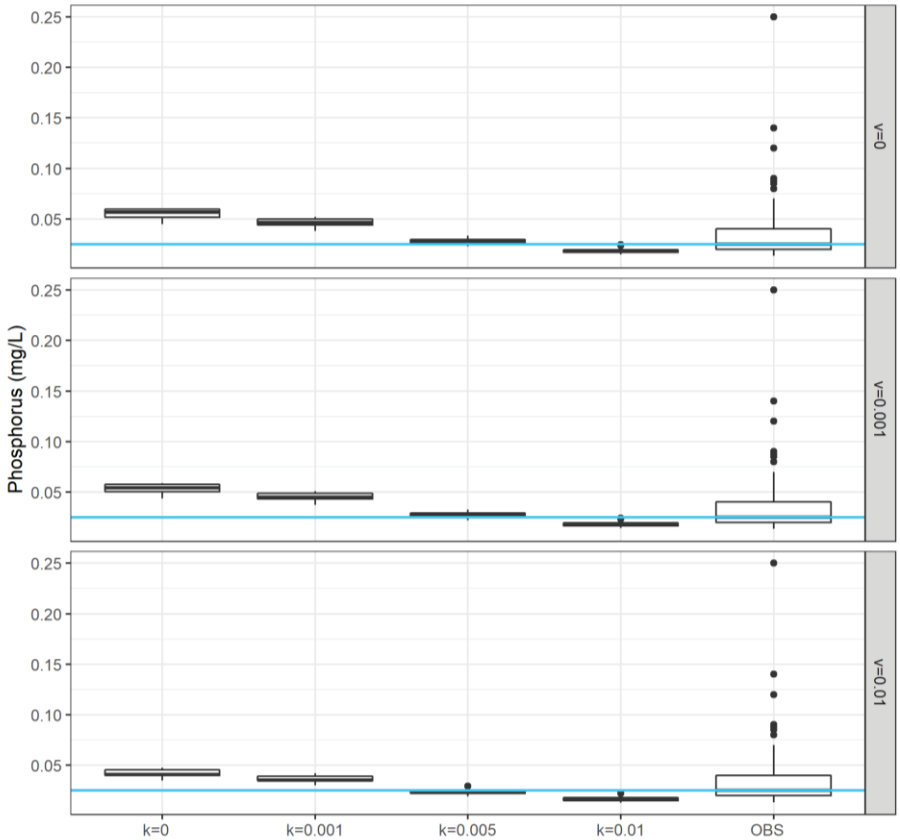
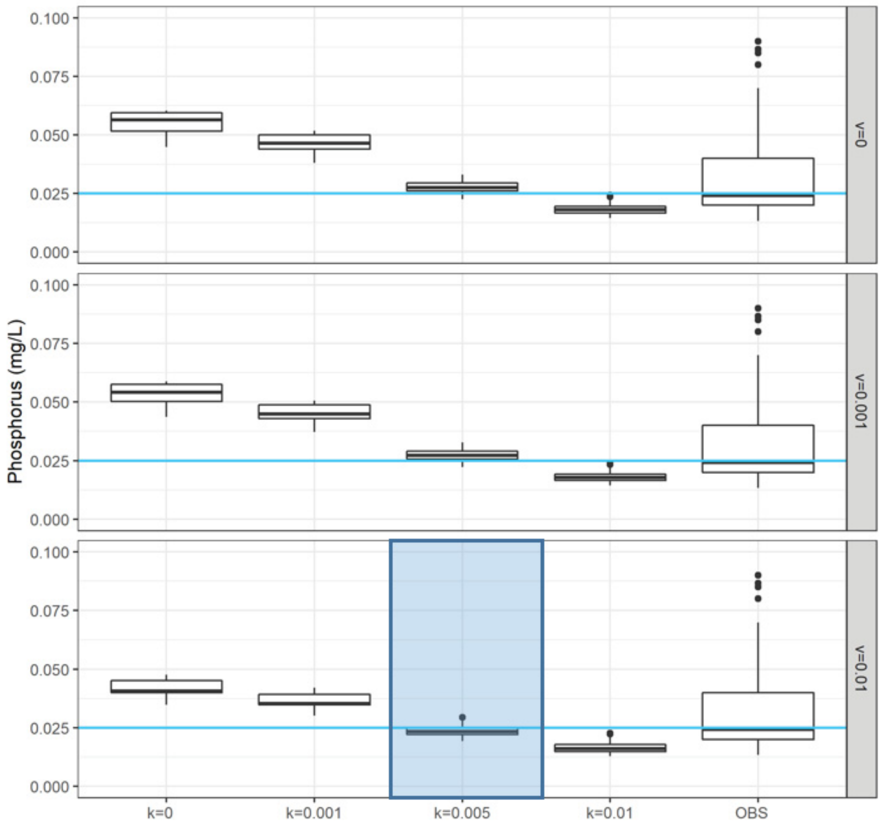


Figure 23 presents the same boxplots with the y axis limited to 0.10 mg/L for better visualization of the boxplots and the median line. The median of the series simulated considering k = 0.005 s^{-1} and v = 0.010 m/s (blue box highlight) is the more similar to the median of observed data (blue horizontal line). Therefore, those parameters values were selected for the model simulations of Jurumirim reservoir.

FIGURE 23 – EXPANDED BOXPLOTS OF THE SENSIBILITY ANALISYS OF THE MODEL PARAMETERS: JURUMIRIM RESERVOIR (THE BLUE LINE REPRESENTS THE MEDIAN OF OBSERVED DATA)



Following the same pattern, Figure 24 presents the calibration boxplots for the Chavantes reservoir. The parameters selected were k = 0.010 s^{-1} and v = 0.010 m/s (blue box highlight), due to the median's similarity to the median of observed data (blue horizontal line).

FIGURE 24 – BOXPLOTS OF THE SENSIBILITY ANALISYS OF THE MODEL PARAMETERS: CHAVANTES RESERVOIR (THE BLUE LINE REPRESENTS THE MEDIAN OF OBSERVED DATA)

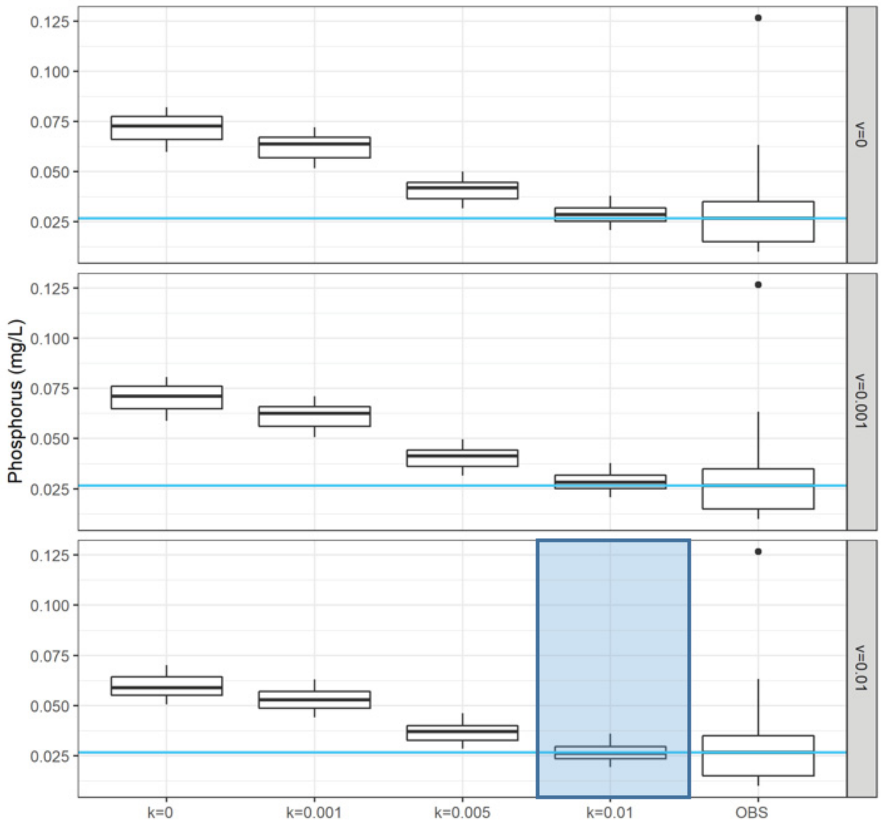
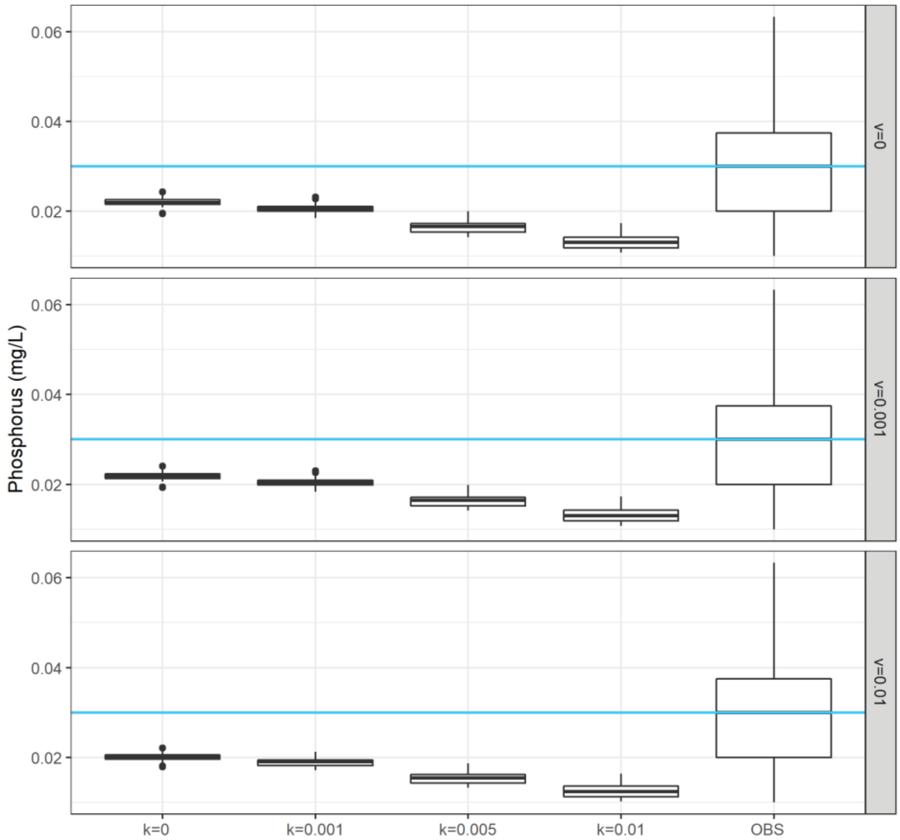


Figure 25 presents the calibration boxplots for the Capivara reservoir. In this case, none of the boxplots were similar to the observed data. Therefore, the same parameters of Chavantes reservoir were selected for the modeling of Capivara reservoir. The parameters selected were k = 0.010 s^{-1} and v = 0.010 m/s.

FIGURE 25 – BOXPLOTS OF THE SENSIBILITY ANALISYS OF THE MODEL PARAMETERS: CAPIVARA RESERVOIR (THE BLUE LINE REPRESENTS THE MEDIAN OF OBSERVED DATA)



A comparison with the parameter k adopted by Toné (2016) for semiarid Brazilian reservoirs ($k = 4/\sqrt{RT}$), by Salas and Martino for tropical reservoirs (1991) ($k = 2/\sqrt{RT}$) and by Vollenweider (1976) for temperate climate ($k = 1/\sqrt{RT}$) is shown in Table 10.

TABLE 10 – COMPARISON OF K VALUES

Reservoir	Residence Time – RT (years)	k (year^{-1}) $4/\sqrt{RT}$	k (day^{-1}) $4/\sqrt{RT}$	k (year^{-1}) $2/\sqrt{RT}$	k (day^{-1}) $2/\sqrt{RT}$	k (year^{-1}) $1/\sqrt{RT}$	k (day^{-1}) $1/\sqrt{RT}$	k (day^{-1}) Present research
Jurumirim	1.071	3.865	0.0106	1.933	0.0053	0.966	0.0026	1.83
Chavantes	0.880	4.264	0.0117	2.132	0.0058	1.066	0.0029	3.66
Capivara	0.350	6.764	0.0185	3.382	0.0092	1.691	0.0046	3.66

The values difference is possibly due to the fact that the aforementioned authors considered a global k and did not consider the sedimentation process (v).

The time series result for each calibration strategy is presented in Figure 26. The figure includes the results of two year simulation (2011 and 2012). The vertical dashed line divides the years in the time axis. The first year (2011) was omitted of further graphics, in order to make sure that the heat up period of the model was not considered in the final results. The simulated series chosen in the calibration phase were highlighted with the arrows colored according to the respective reservoir.

FIGURE 26 – TIME SERIES OF THE SENSIBILITY ANALISYS OF THE MODEL PARAMETERS (K: S^{-1} AND V: M/S) – JURUMIRIM, CHAVANTES AND CAPIVARA RESERVOIRS

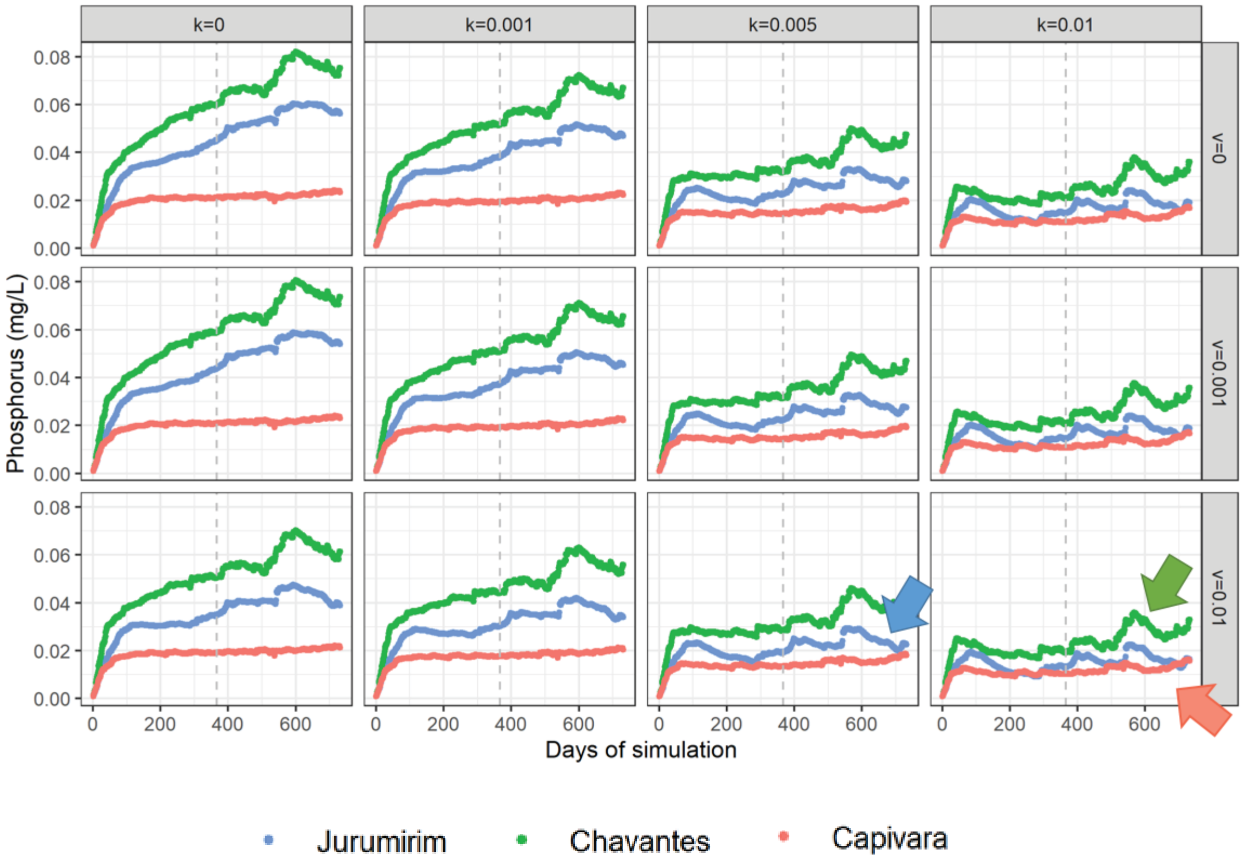


Figure 26 also works as a sensibility test for the k and v parameters. The smaller the parameters are, the bigger the phosphorus concentration is, since the terms of reaction and sedimentation are reduced.

The input synthetic series and output modeled concentrations of the year 2012 are shown in Figure 27. The synthetic series (input) has more variation in their values, since the numbers are generated in a partially deterministic autoregressive process, in which the following value is proportional to the previous one, but there is the statistical noise. The output concentrations, on the contrary, are continuous series, since the generated number is always a function of the previous value. The dashed horizontal line is the Class 2 CONAMA limit. For better visualization, the output concentrations for the year 2012 are presented individually in Figure 28.

FIGURE 27 – INPUT AND OUTPUT PHOSPHORUS CONCENTRATIONS: BASE SCENARIO (THE DASHED HORIZONTAL LINE IS THE CLASS 2 LIMIT).

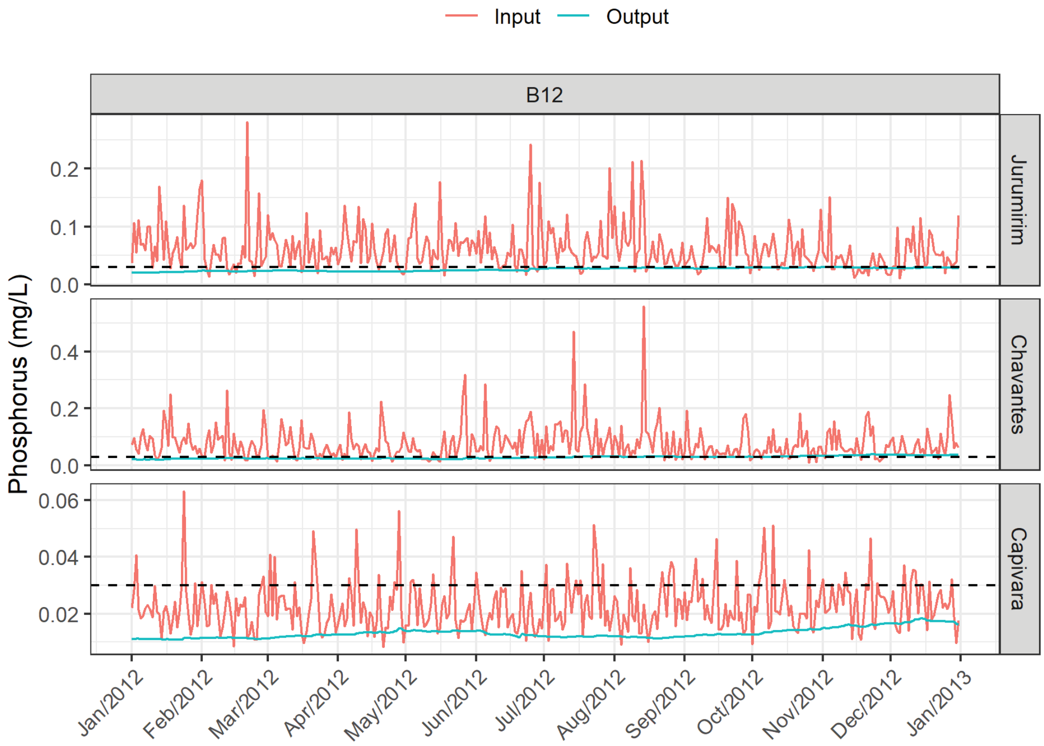
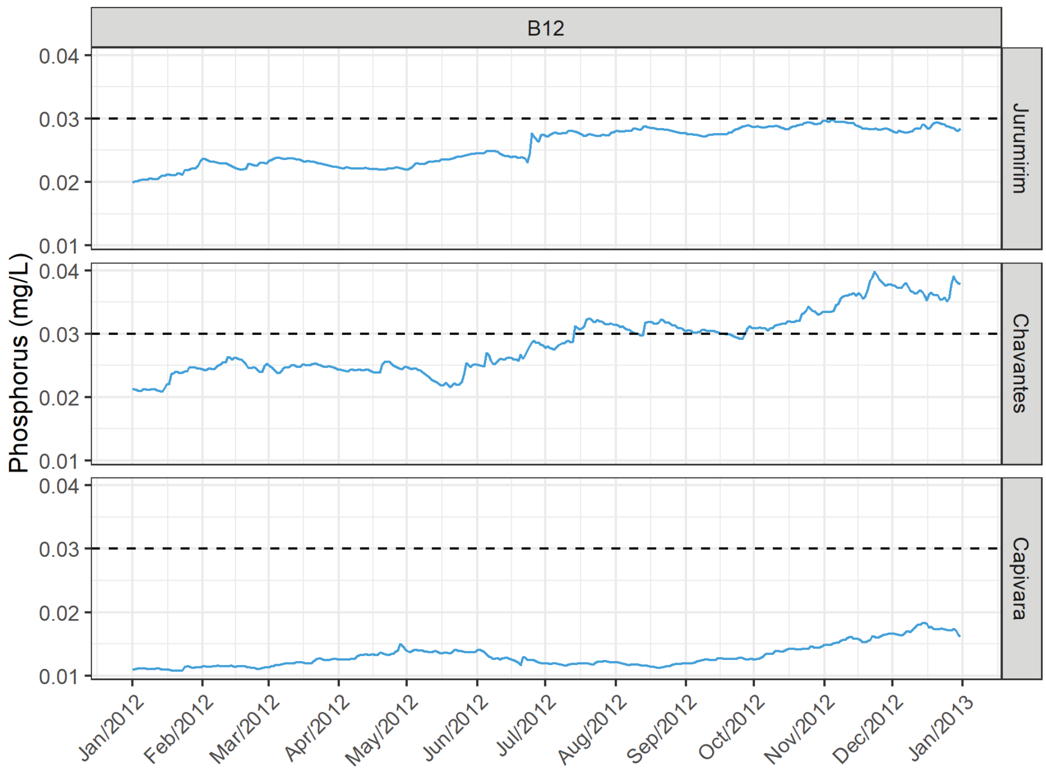


FIGURE 28 – OUTPUT PHOSPHORUS CONCENTRATIONS: BASE SCENARIO (THE DASHED HORIZONTAL LINE IS THE CLASS 2 LIMIT).



For the reference scenario (B12) (Figure 28), only the Chavantes reservoir presented values above the CONAMA resolution limit for Class 2 of 0.03 mg/L. Jurumirim and Capivara results were below that limit. The increase in the phosphorus concentrations that happened in June and July at the reservoirs Jurumirim e Chavantes reflect the flow values occurred in that period. The inflow and outflow series of each reservoir are exhibited in Figure 29. Those values can help in the interpretation of some aspects of the output concentration series.

FIGURE 29 – INFLOW AND OUTFLOW OF THE MODEL

Figure 30 shows the input and output concentrations for all scenarios described in Table 7. The input synthetic series concentrations grow as the sceneries become more critic. The dashed horizontal line is the Class 2 CONAMA limit. For better visualization, the output concentrations are presented individually in Figure 31.

In Jurumirim reservoir, the output concentrations only stand below the limit concentration in B12 scenery. In T25, A25, T35 and A35, all the values were higher than the limit. For Chavantes reservoir, the output concentrations are also above the limit in the T25, A25, T35 and A35 sceneries. Capivara reservoir stands below the limit most of the days in the scenaries B12, T25, A25 and T35. However, in A35 all values are above the limit.

FIGURE 30 – INPUT AND OUTPUT PHOSPHORUS CONCENTRATIONS: BASE, TENDENTIAL AND ACCELERATED SCENARIOS (THE DASHED HORIZONTAL LINE IS THE CLASS 2 LIMIT).

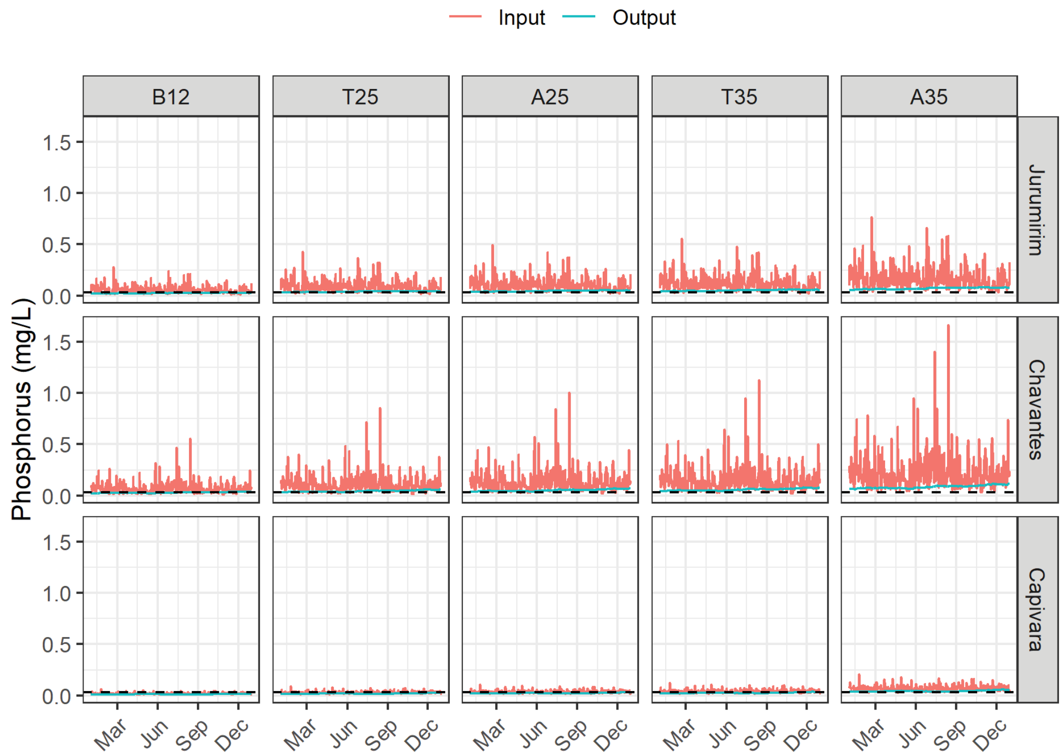


FIGURE 31 – OUTPUT PHOSPHORUS CONCENTRATIONS: BASE, TENDENTIAL AND ACCELERATED SCENARIOS (THE DASHED HORIZONTAL LINE IS THE CLASS 2 LIMIT)

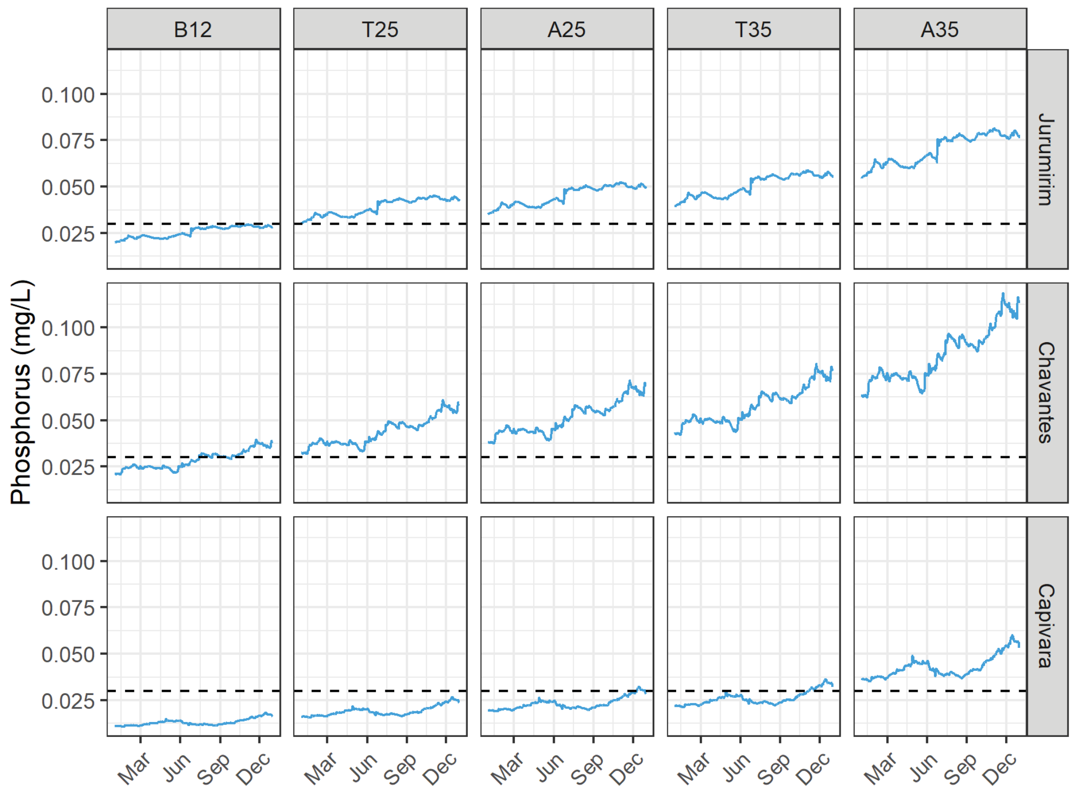


Figure 32 present the same results in logarithmic scale, compared to the TSI limits. Figure 33 and Figure 34 show the same information in sectors graphics, so that is possible to evaluate the proportion that a particular class happened during the simulated year.

The input synthetic concentrations (Figure 33) varied from ultraoligotrophic to hypereutrophic in Jurumirim and Chavantes reservoir and from ultraoligotrophic to eutrophic in Capivara Reservoir.

Regarding the output simulated concentrations results (Figure 34), it has been noted that they are more continuous and lower than the input synthetic series concentrations. It reinforces the reservoir role in decreasing the pollutants concentrations downstream. The reason for that is that the decrease in water velocity and increase in retention time favor the occurrence of chemical and biological oxidation and decantation of various elements in the sediments, of which phosphorus is one of the most susceptible, as stated by Cunha-Santino et al. (2017). Zubala (2009) also points out the reservoir role in the processes of self-purification that improves the quality of waters flowing out of anthropogenically transformed areas.

In Jurumirim reservoir, in B12 all results were in the oligotrophic classification. In T25, this class occurred in only 4% of the time. In the rest of the year, data was classified in mesotrophic state. In A25, T35 and A35 sceneries, all data were classified in mesotrophic state.

In Chavantes reservoir, the classification varied from oligotrophic to mesotrophic as well. In B12 and T25, 22% and 0.3% of the results were oligotrophic, respectively. In A25, T35 and A35 sceneries all data was mesotrophic.

In Capivara reservoir, in B12, 35% of the year presented ultraoligotrophic results and the other 65% of the year concentrations were oligotrophic. In T25, A25 and T35, 100%, 99% and 89% of the results were oligotrophic, respectively. In A35, all results were mesotrophic.

FIGURE 32 – INPUT AND OUTPUT PHOSPHORUS CONCENTRATIONS AND TROPHIC STATE INDEX (TSI)

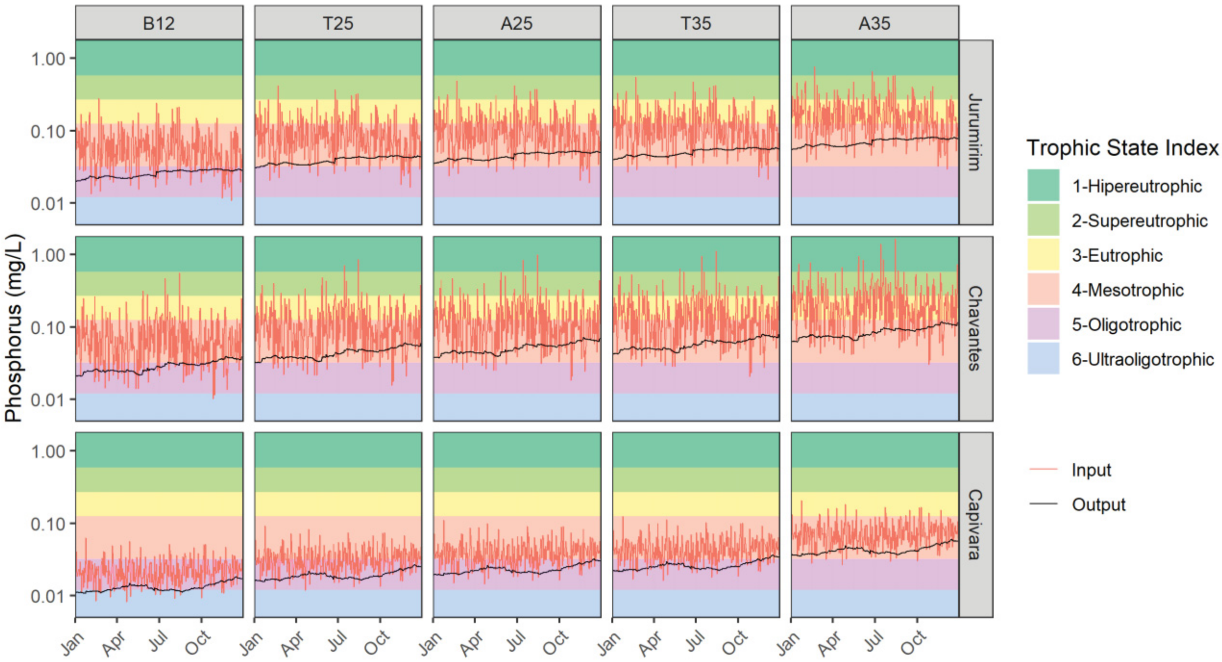


FIGURE 33 – TROPHIC STATE INDEX OF THE INPUT PHOSPHORUS CONCENTRATIONS

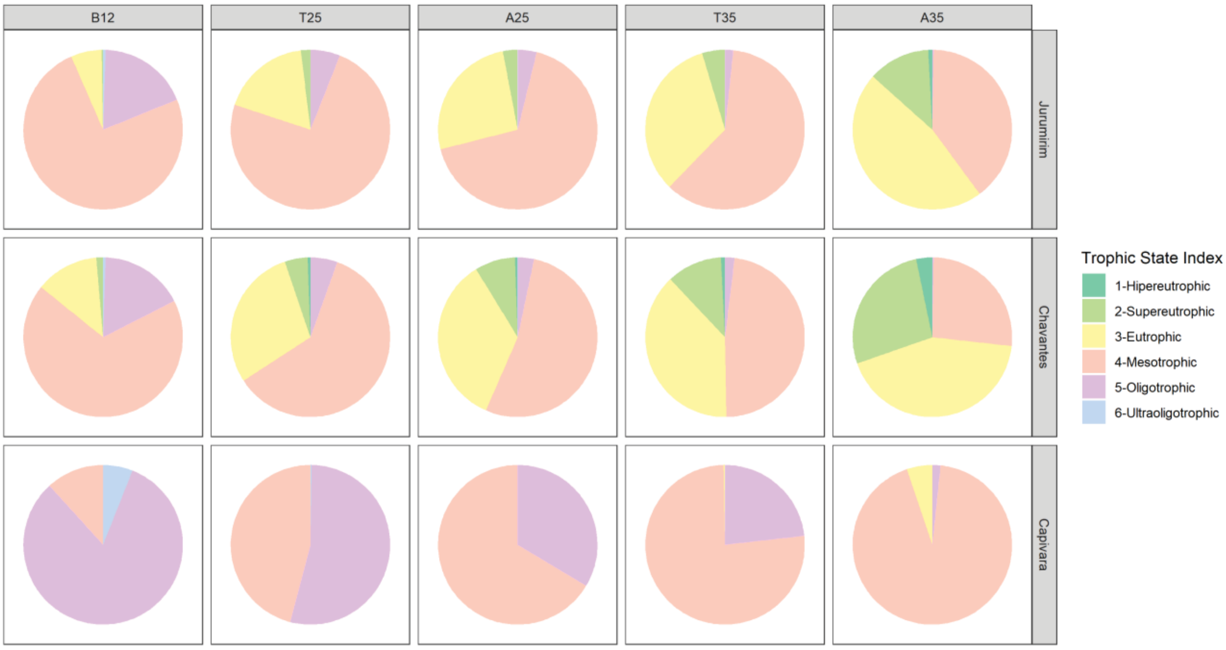


FIGURE 34 – TROPHIC STATE INDEX OF THE OUTPUT PHOSPHORUS CONCENTRATIONS

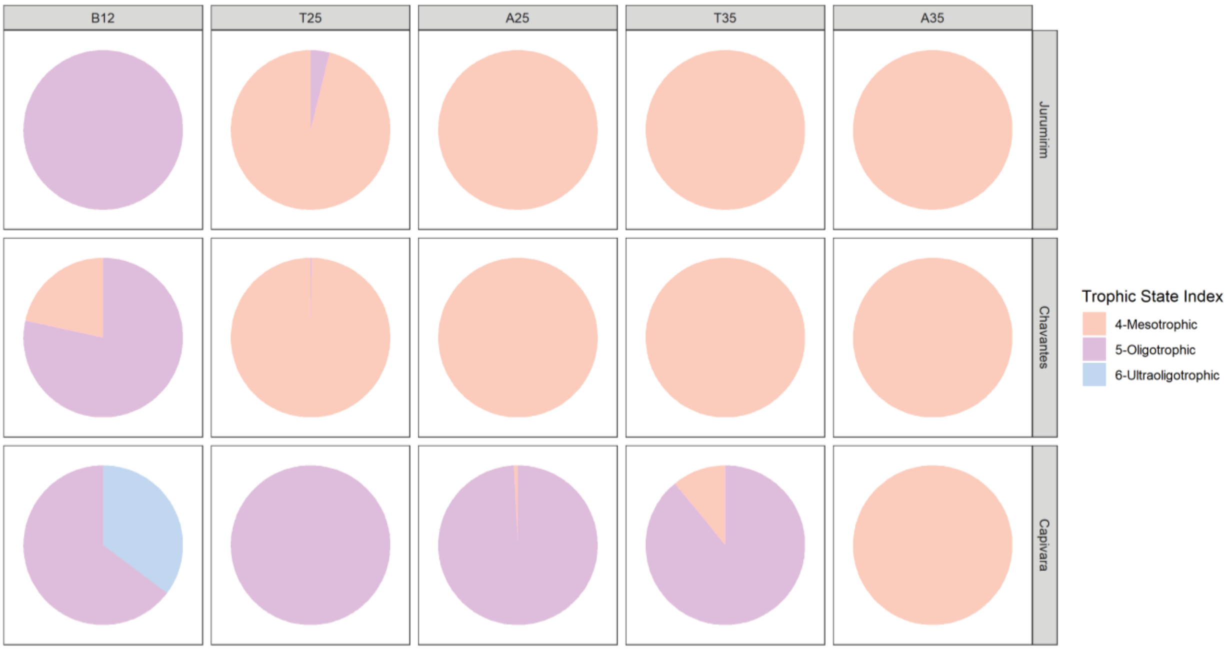


Figure 35 and Figure 36 show the load duration curves in the entry and in the exit of the reservoir, respectively. As can be seen in the y axis, the magnitude of the values are reduced considerably in the outlet. These values were compared to the TMDLs correspondent to the same flow (input limit and output limit).The shape of the outlet load duration curves was defined by the pattern of the regulated flow considering the reservoir operation (Figure 29).

FIGURE 35– LOAD DURATION CURVES IN THE RESERVOIRS INLET

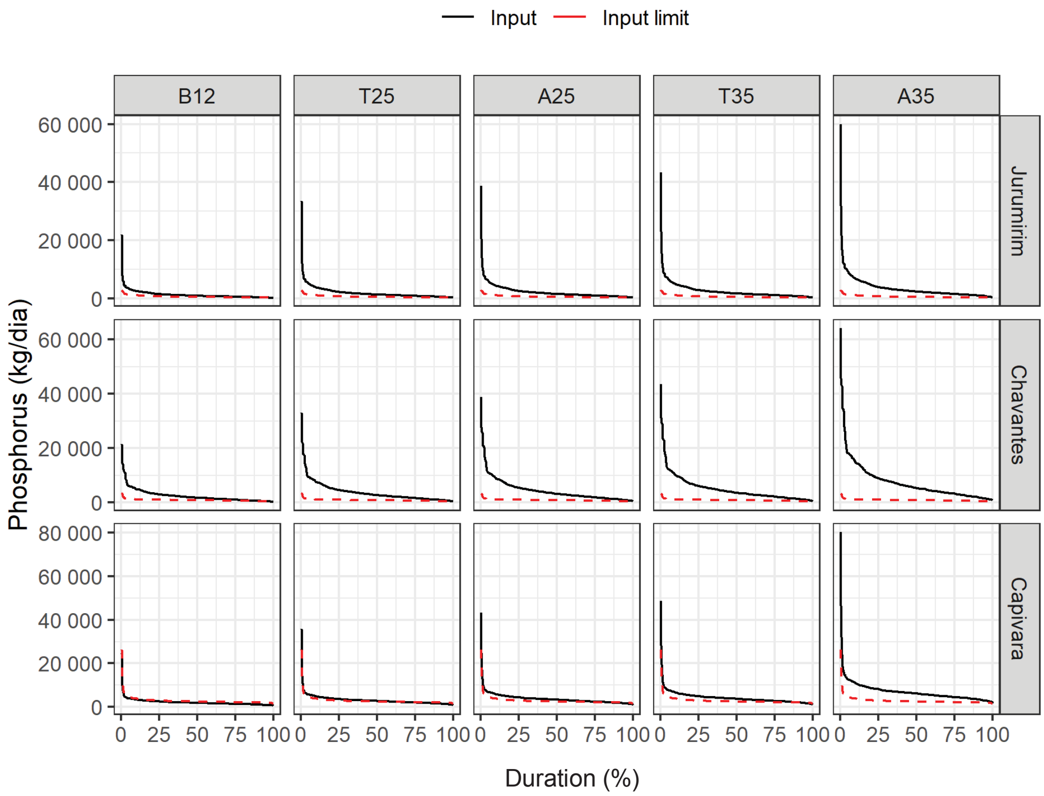
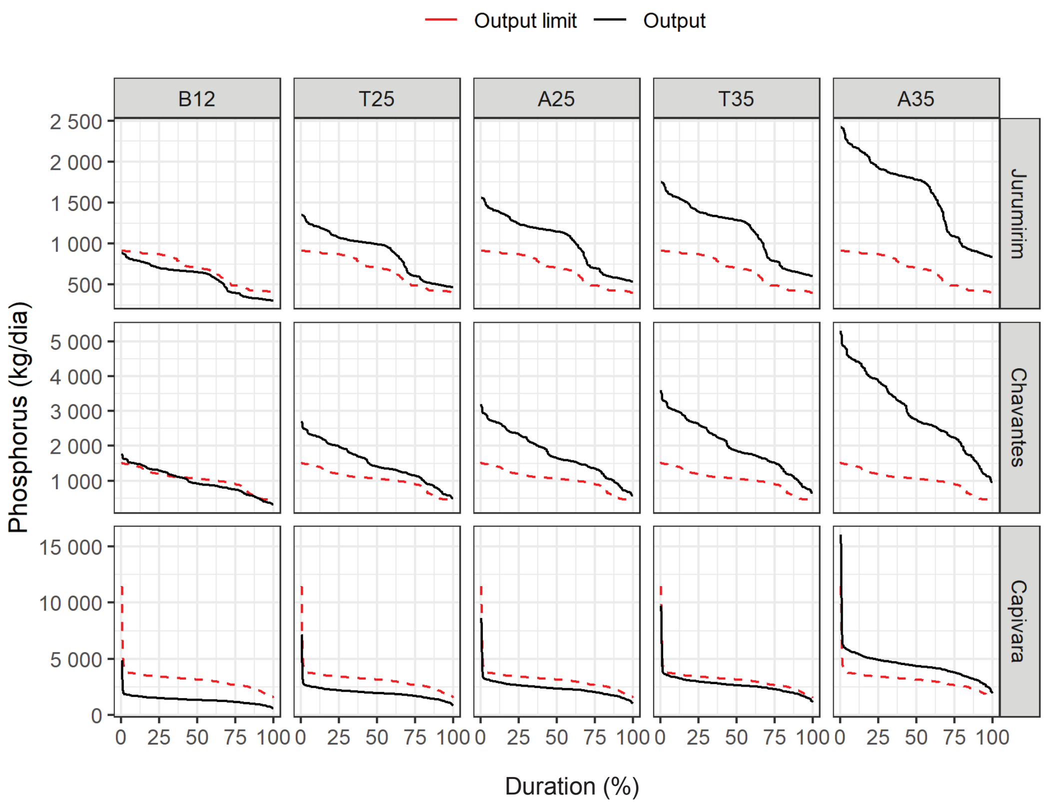


FIGURE 36 – LOAD DURATION CURVES IN THE RESERVOIRS OUTLET



The Total Maximum Daily Loads were calculated as the mean of the daily load results of model B. Figure 37 indicated that the TMDLs are above the class 2 limit in all economic scenarios. The Total Maximum Annual Loads, which corresponds to the sum of the daily loads, are showed in Figure 38.

FIGURE 37 – TOTAL MAXIMUM DAILY LOADS FOR CLASS 2 LIMITS

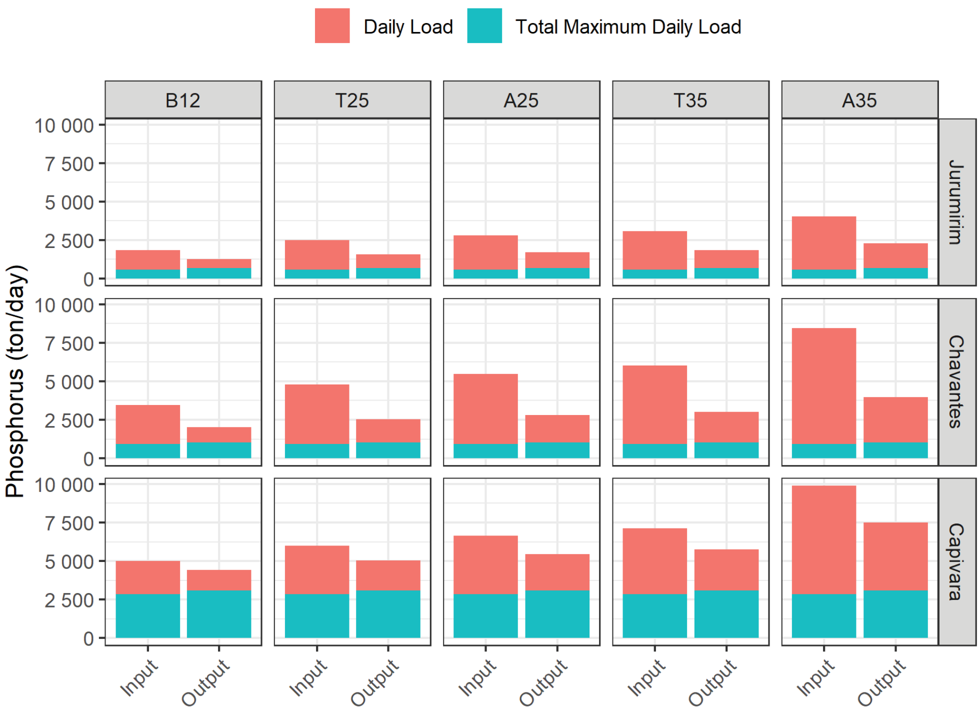
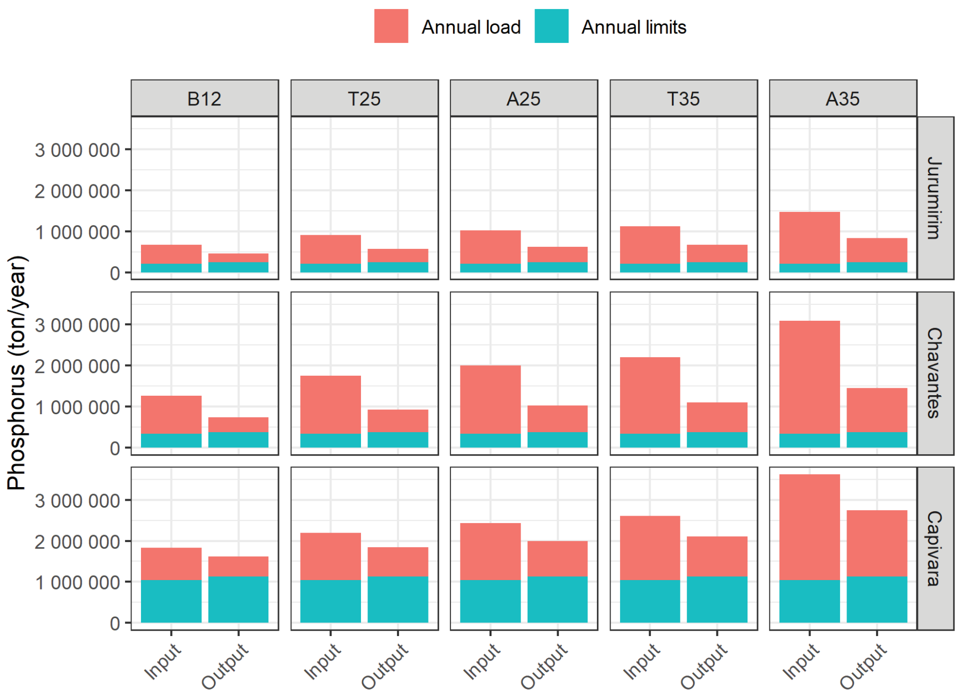


FIGURE 38 – TOTAL MAXIMUM ANUAL LOADS FOR CLASS 2 LIMITS



4.4 MODEL C – UNSTEADY FLOW STATE WITH COMPARTMENTS

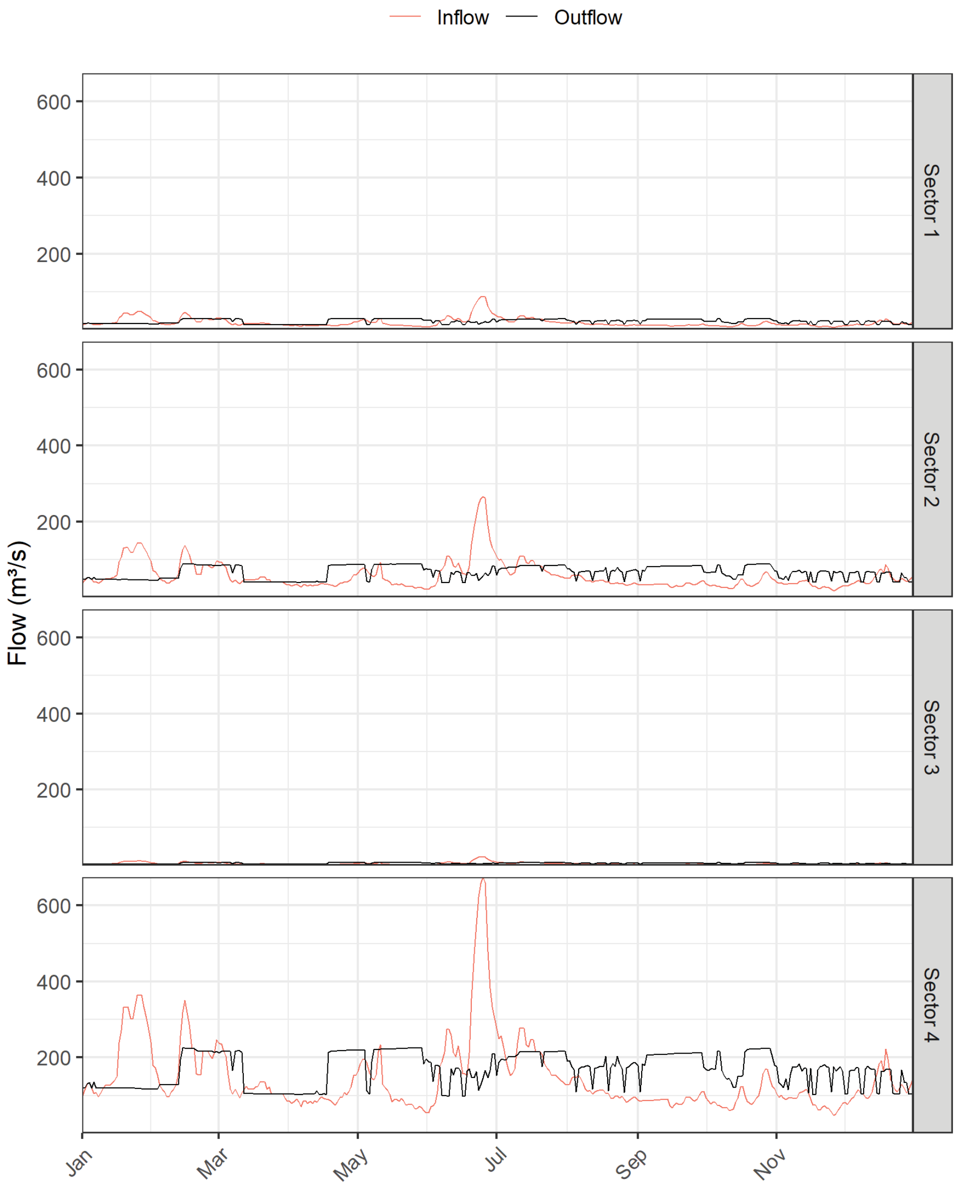
In this item, the zero-dimensional unsteady CSTR model is applied to the four sectors of the Jurumirim reservoir, as explained in topics 3.5 and 3.8. The first step was to estimate the flow and concentration series for each sector, as explained below.

The flow series of the sectors was estimated based on the flow series of the inflow and outflow of the reservoir. In order to divide the flow of the reservoir between the sectors, it was considered that each sector received a percentage of the flow. This proportions were defined as functions of the drainage area of the tributaries of each sector. Table 11 shows the proportions of the areas, which were applied to the calculations of the flow series of the sectors (Figure 39).

TABLE 11 – PROPORTOINS OF THE DRAINAGE AREAS OF EACH SECTOR OF JURUMIRIM RESERVOIR

Sector	Proportion of the area
Sector 1 (Dam)	8,4%
Sector 2 (Taquari)	25,3%
Sector 3 (Ribeirão das Posses)	2,3%
Sector 4 (Paranapanema)	64,0%
Total	100,0%

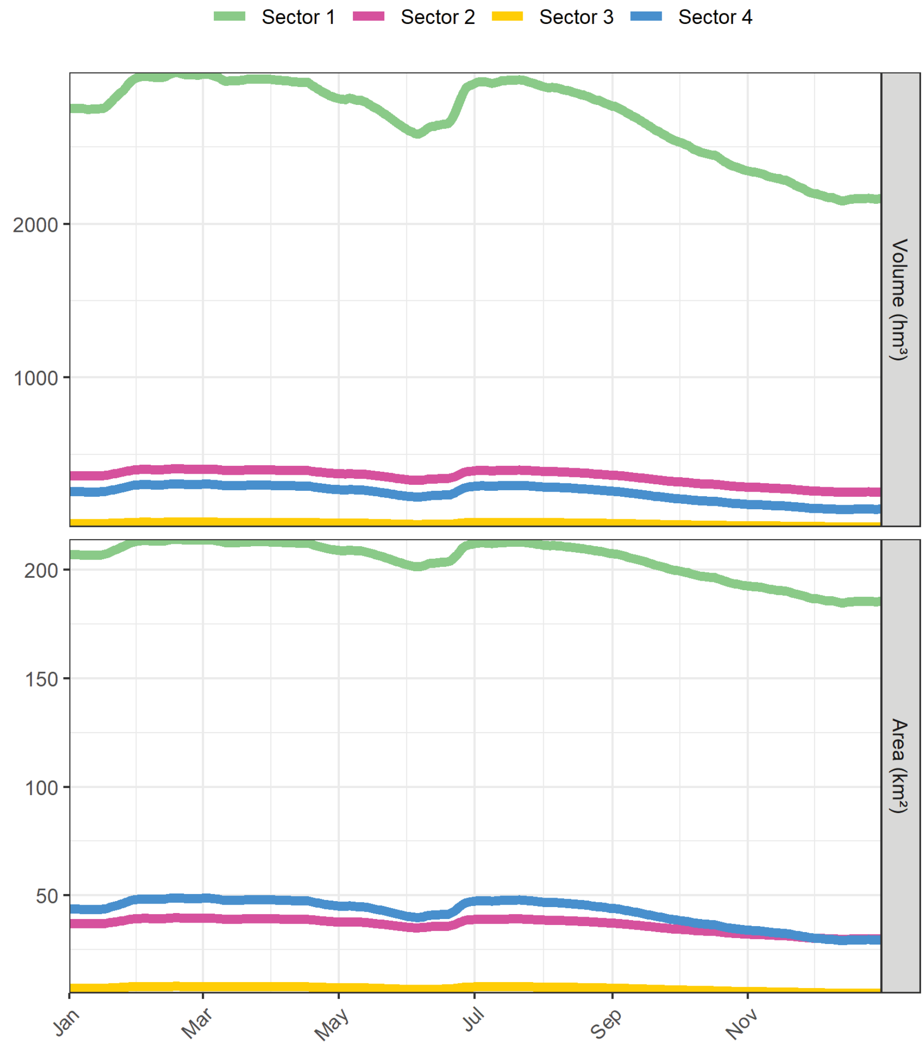
FIGURE 39 – INFLOW AND OUTFLOW OF THE FOUR SECTORS OF JURUMIRIM RESERVOIR



The estimation of the load series followed the same process. The synthetic load series was given by the concentration of the synthetic series applied on item 4.3 multiplied by the area proportions (Table 11) and to the flow (Figure 39). Then, the concentrations were obtained from the loads by the inverse process (dividing by the flow).

The volumes and areas were obtained by an algorithm that considers the bathymetry and the water level of the reservoir. The resulting volume and area time series were presented in Figure 40. It is worth to take into account the fact that this estimation presented some imprecisions, since the sum of the sectors volumes and areas did not corresponded to the whole reservoir volume and area.

FIGURE 40 – VOLUMES AND AREAS FOR EACH SECTOR OF JURUMIRIM RESERVOIR



The input synthetic series and the output of the model are exhibited in Figure 41. The phosphorus axis is in logarithmic scale.

In sector 1, which represents the final concentrations on the outlet of the reservoir, the results were classified from mesotrophic to eutrophic categories.

In sector 2 (Taquari), in B12, the outlet values were classified as oligotrophic and mesotrophic, while in T25, A25, T35 and A35 the reservoir was classified mainly in the mesotrophic category.

The sector 3 (Ribeirão das Posses) presented the more critical Trophic State Index when compared to the other sectors. It varied form eutrophic to hypereutrophic states. In A35, for example, 96% of the data was in hypereutrophic state.

Sector 4 (Paranapanema) output concentrations varied from oligotrophic state to supereutrophic state.

Figure 42 and Figure 43 exhibit the proportions of time that each of the trophic states occurred.

FIGURE 41 - INPUT AND OUTPUT PHOSPHORUS CONCENTRATIONS AND TROPHIC STATE INDEX (TSI) APPLIED TO THE FOUR SECTORS OF JURUMIRIM RESERVOIR

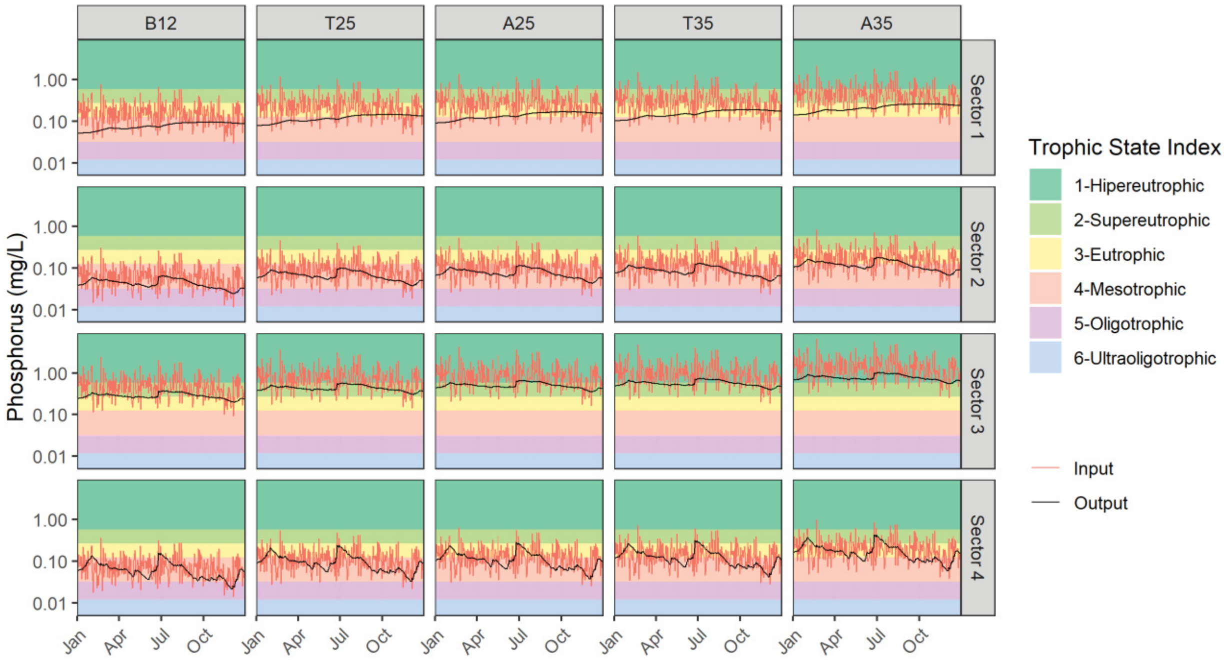


FIGURE 42 – TROPHIC STATE INDEX OF THE INPUT PHOSPHORUS CONCENTRATIONS

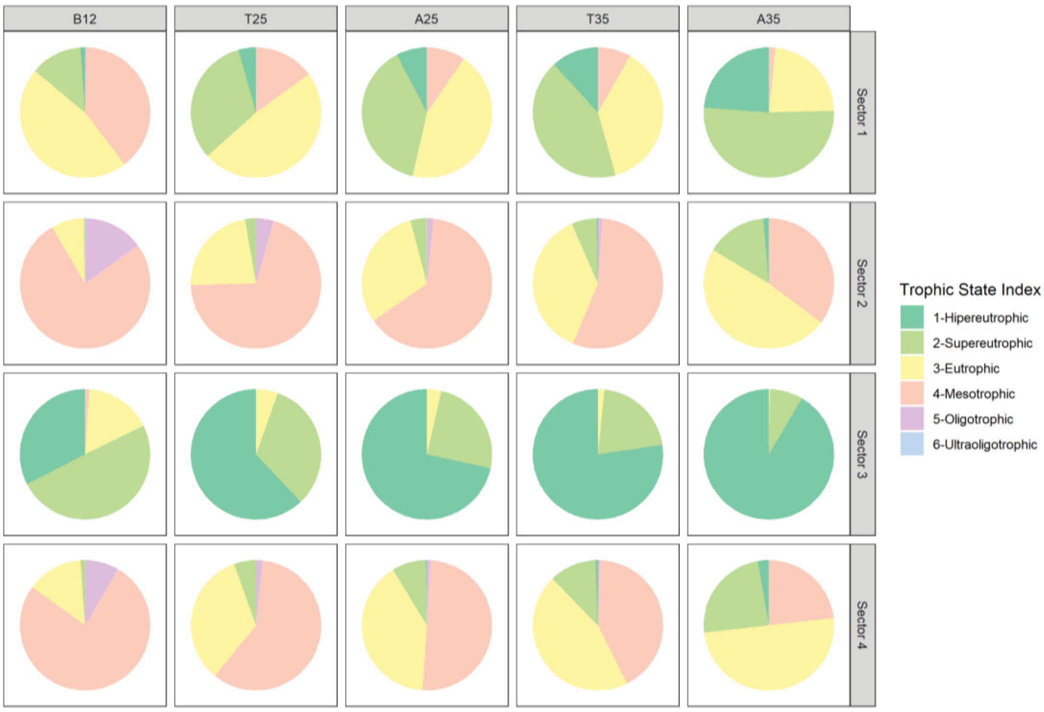


FIGURE 43 – TROPHIC STATE INDEX OF THE OUTPUT PHOSPHORUS CONCENTRATIONS

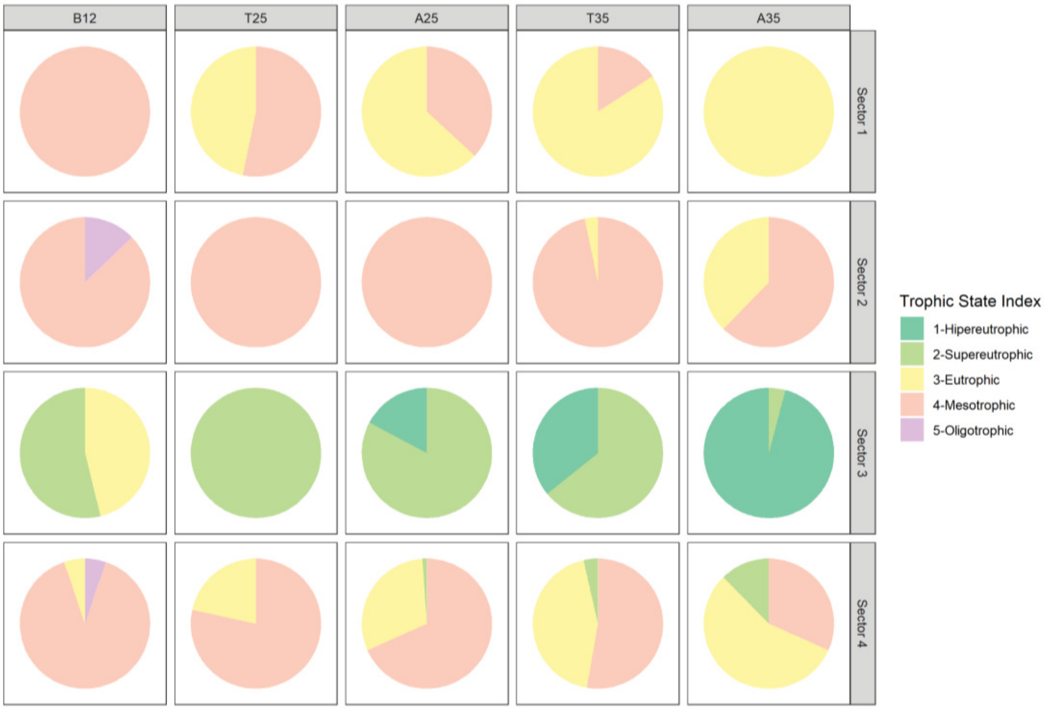
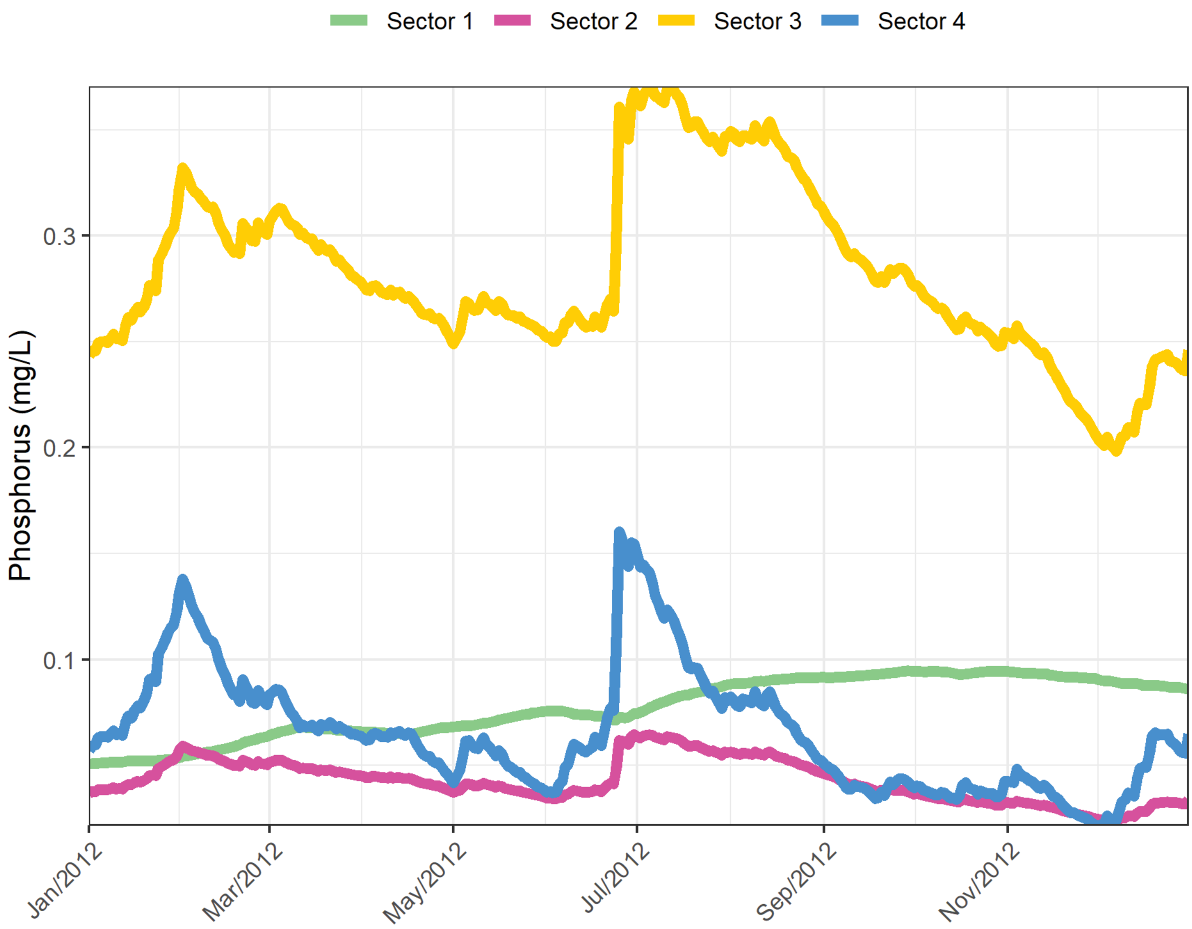


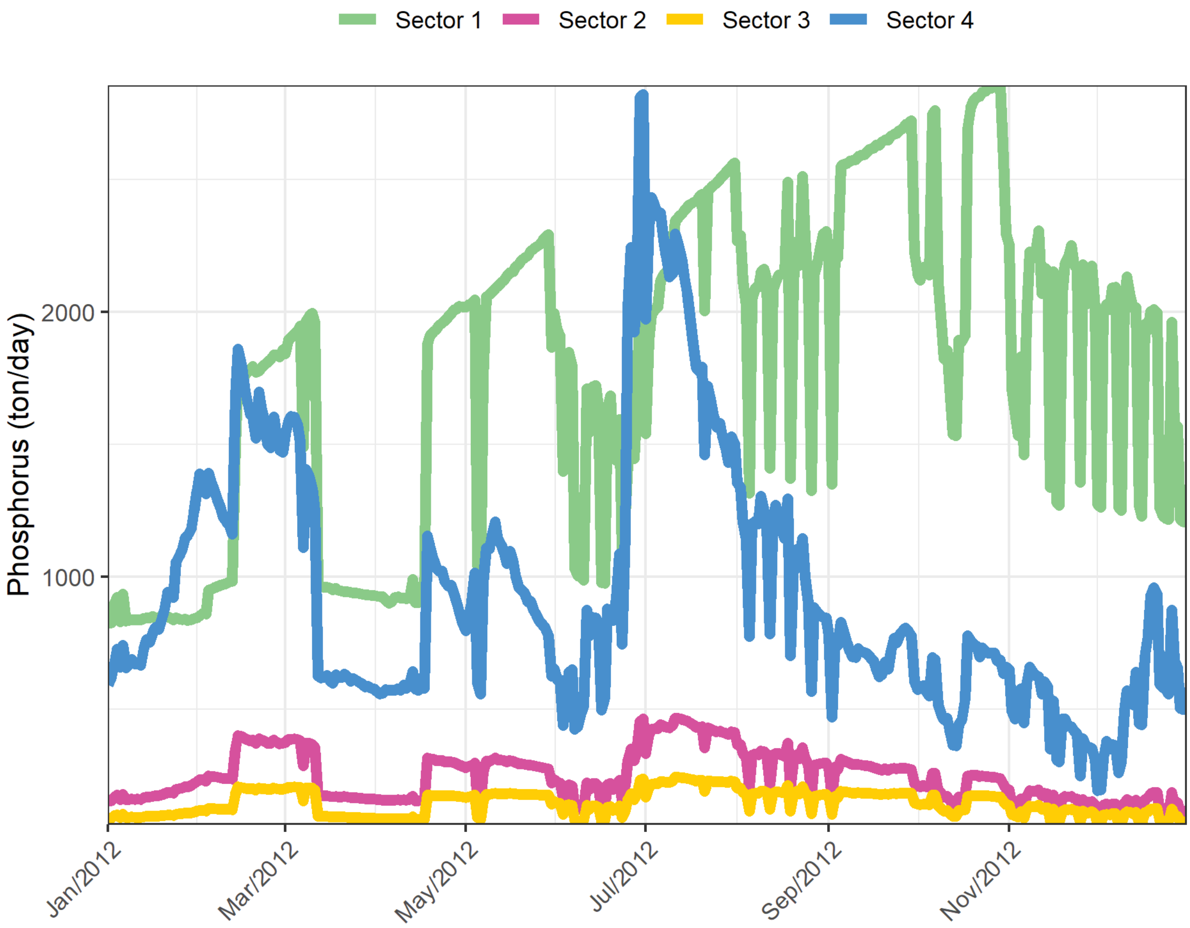
Figure 44 provides a comparison of the output time series of the sectors for the year 2012 (B12 scenario). Sector 3 (Ribeirão das Posses) has the most expressive phosphorus concentrations, which exceed 0.3 mg/L. In sector 2 (Taquari) and sector 4 (Paranapanema), most of the values were below 0.15 mg/L. The sector closer to the dam (sector 1) considers the other sector's concentration as input values. Thus, the variation in the time series is smaller.

FIGURE 44 – PHOSPHORUS CONCENTRATIONS IN THE FOUR SECTORS OF JURUMIRIM RESERVOIR



Regarding the load time series (Figure 45), the sector 3 no longer present the highest values. Although the high concentrations are in that location, its contribution to the reservoir is minor due to smaller flows. The highest loads are in the sector 1 (closer to the dam), followed by sector 4. The contributions of sector 2 and sector 3 are not as significant as the load of the main river.

FIGURE 45 – PHOSPHORUS LOADS IN THE FOUR SECTORS OF JURUMIRIM RESERVOIR



4.5 COMPARISON OF THE ZERO-DIMENSIONAL MODELS WITH A THREE-DIMENSIONAL MODEL

The results of the zero-dimensional models and Delft3D model were compared below. Model B concentrations for the scenery B12 varied from 0.020 to 0.030 mg/L, while model C concentrations varied from 0.050 mg/L to 0.095 mg/L. The concentrations from model Delft3D varied from 0.055 mg/L to 0.070 mg/L. Figure 46 compares the time series of the three models in the scenery B12. In all scenarios, model C average was 3 times higher than model B average and 1.2 times higher than Delft3D average.

Regarding the phosphorus limits, the results of all models exceeded Class 1 limit (0.02 mg/L). Model B and Delft3D results exceeded the Class 3 limit (0.05 mg/L) in the whole simulated time. In Figure 46, the horizontal dashed lines illustrate the abovementioned limits.

In terms of load, the difference between the models can be seen as well (Figure 47). For comparison purposes, the means of the three models were higher than the Class 1 TMDL (420 ton/day), and the mean of Model C and Delft3D results were higher than Class 2 and Class 3 TMDLs (630 ton/day and 840 ton/day, respectively).

The average concentrations and loads of all scenarios are exhibited in Table 12.

FIGURE 46 – COMPARISON OF THE CONCENTRATIONS OF ZERO-DIMENSIONAL MODELS AND DELFT3D – THE HORIZONTAL DASHED LINES ILLUSTRATE THE PHOSPHORUS LIMITS FOR CLASSES 1, 2 AND 3 FOR JURUMIRIM RESERVOIR.

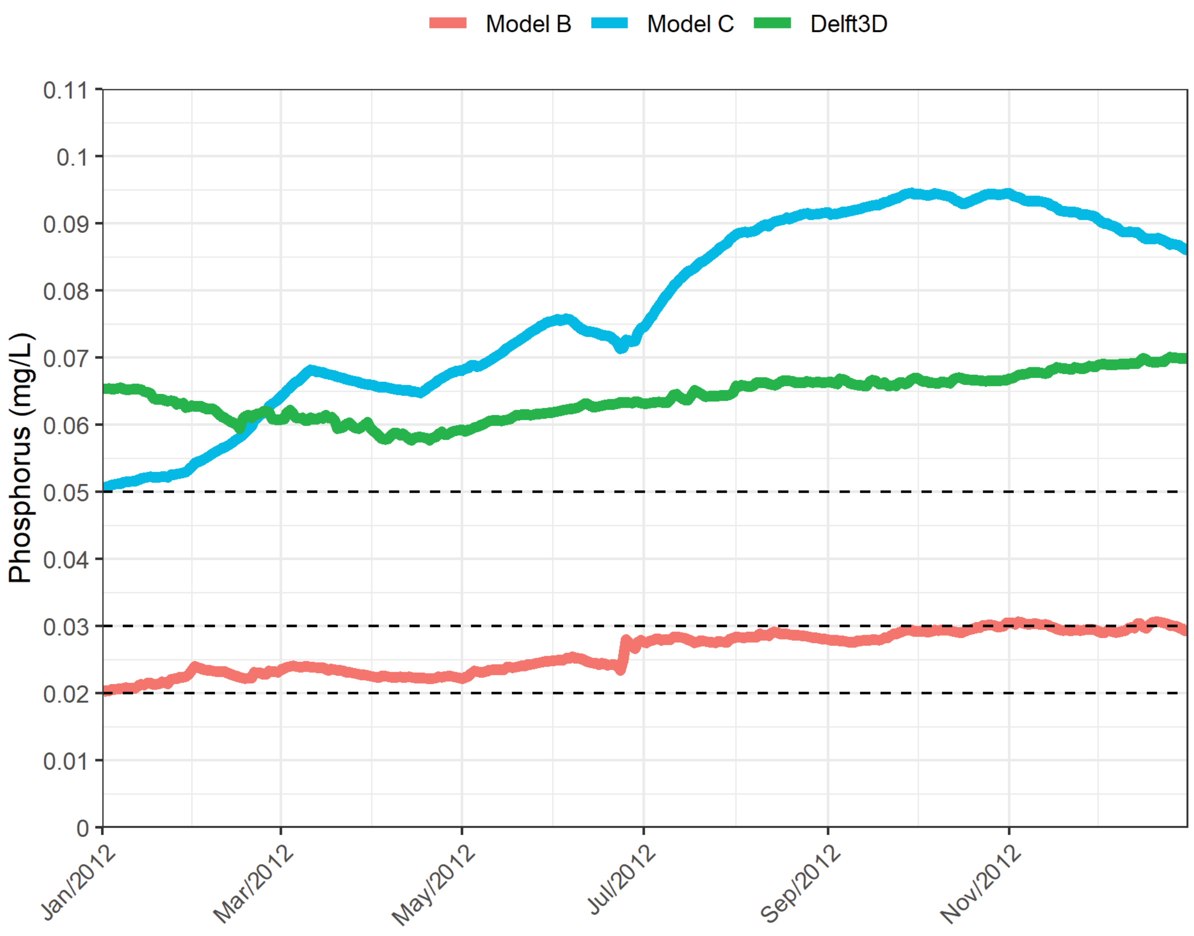


FIGURE 47 – COMPARISON OF THE LOADS OF ZERO-DIMENSIONAL MODELS AND DELFT3D FOR JURUMIRIM RESERVOIR

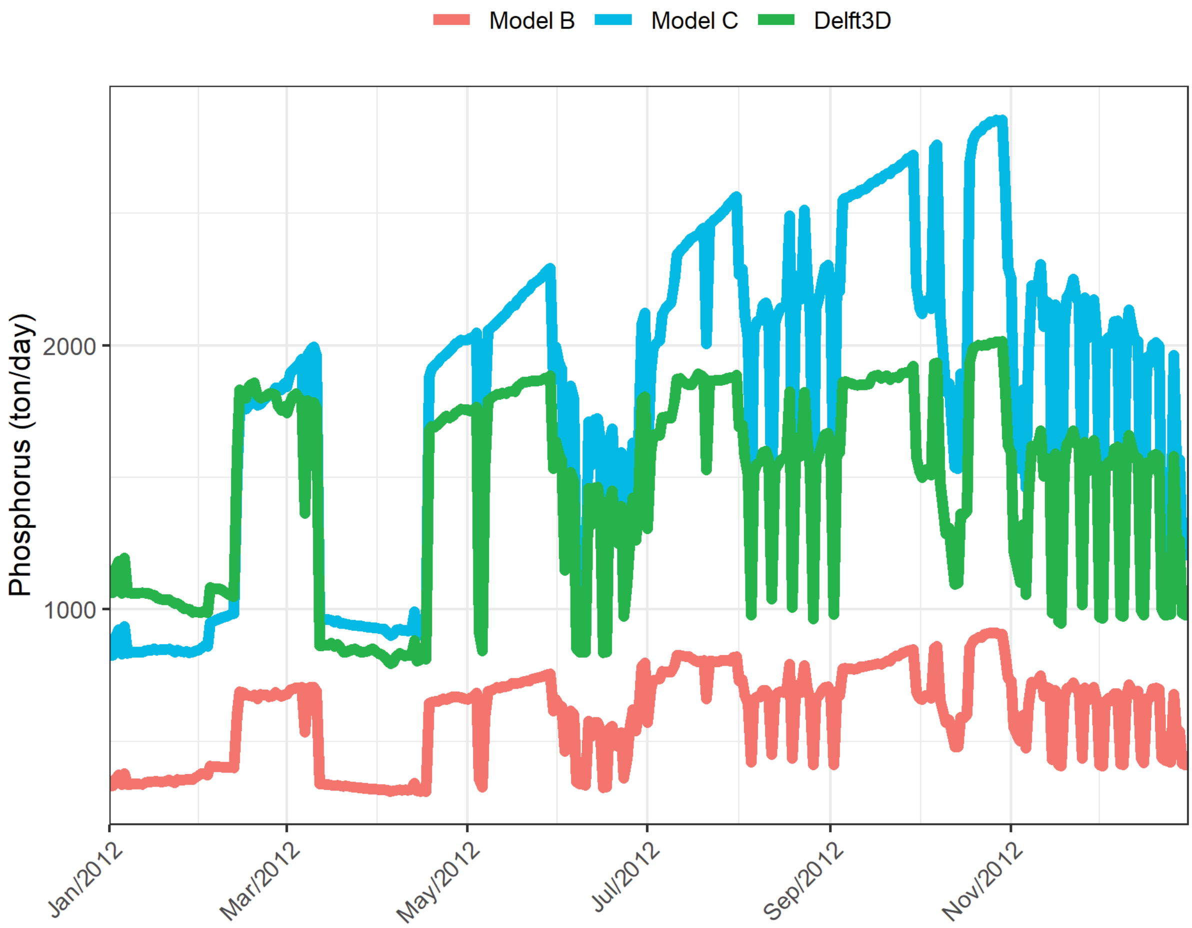
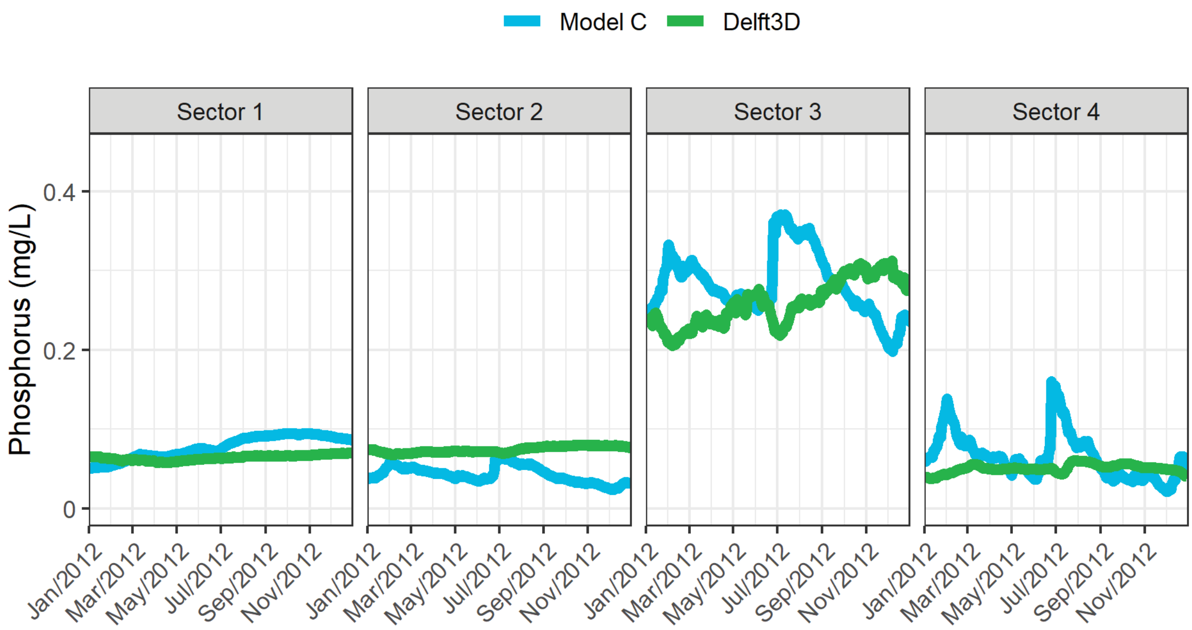


TABLE 12 – COMPARISON OF MODEL B, MODEL C AND THE THREE-DIMENSIONAL MODEL FOR JURUMIRIM RESERVOIR

Scenery	Average concentration (mg/L)			Average load (ton/day)		
	Model B	Model C	Delft3D	Model B	Model C	Delft3D
B12	0.026	0.077	0.064	599	1785	1458
T25	0.040	0.118	-	913	2724	-
A25	0.046	0.137	-	1055	3150	-
T35	0.052	0.153	-	1183	3533	-
A35	0.072	0.212	0.164	1637	4887	3743

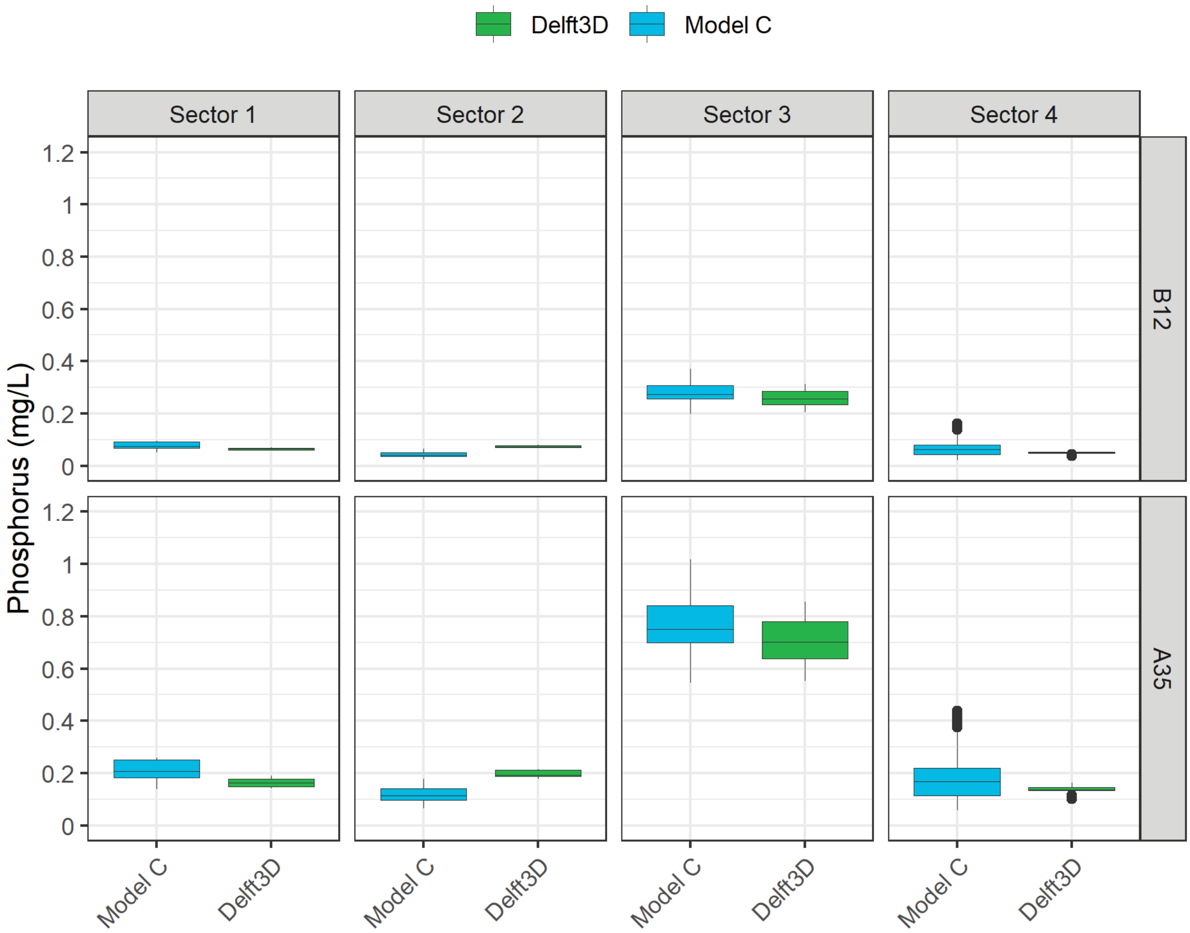
The time series of the result of each sector for the scenery B12, comparing the model C with Delft 3D are expressed in Figure 48. The magnitude of the concentrations simulated for Jurumirim reservoir sectors was similar for both models. The behavior throughout the time, however, is distinct.

FIGURE 48 – COMPARISON OF MODEL C AND DELFT3D – SECTORS – TIME SERIES FOR JURUMIRIM RESERVOIR



The boxplots in Figure 49 reinforce that the order of magnitude was similar for the sceneries B12 and A35, which presented the smallest and the biggest phosphorus concentrations, respectively.

FIGURE 49 – COMPARISON OF MODEL C AND DELFT3D – SECTORS – BOXPLOT FOR JURUMIRIM RESERVOIR



Although the simulated series are numerically different (Figure 46), in the point of view of planning and management of reservoirs, the magnitude of the values can be considered similar. Despite some concentrations exceeded the legislated limits, Paranapanema watershed presents low phosphorus concentrations when compared to more polluted regions. In Iguaçu river, for example, phosphorus values above 1.5 mg/L were found by Knapik (2009). The proposed 0D model with sectors (model C) is able to show the differences of the four regions, even though the lower values such as the series of sector 1 and 2 are different from the 3D model. In future studies, it is recommended to apply this model to more polluted reservoirs in order to check whether or not the sectors present prominent differences.

5 FINAL REMARKS

"If you cannot do great things, do small things in a great way."
- Napoleon Hill

The present research contributes to the challenge of simplifying the modeling processes. The results obtained for model C (reservoir modelled with sectors) were in the same magnitude of the results of a 3D simulation and fulfilled the goal of applying a 0D model in the case study of Jurumirim reservoir. The 0D simulation with sectors was capable of identifying the reservoir region that outstands in the context of planning and management (Sector 3 – Ribeirão das Posses).

The similar results of the zero-dimensional (0D) and three-dimensional (3D) models show the simplified numerical schemes are important potential tools to be considered for initial analysis of water quality dynamics in reservoirs and for management purposes. It is recommended that more studies are made in this context in order to consolidate the quality and the equivalency of the simulated results.

One possible reason that justify the difference of models B and C results can be the simplification of the flows and concentrations distribution based on the drainage area. The verification of the mass balance of each sector may contribute to this aspect of future applications of the 0D model in reservoir sectors. In addition, the calculation method of areas and volumes of each sector presented some imprecisions. These imprecisions possibly led to overestimation of the concentration results of model C (reservoir modelled with sectors).

Another simplification adopted in this study was the same first order decay coefficients (k) and apparent settling velocities (v) for all sectors. In future applications, it can be improved based on the morphological characteristics of each sector. In Sector 1, for example, these parameter values can be modified in order to represent the strongest lentic characteristics of this region. Besides, due to the uncertainties in the definitions of those parameters, it may be helpful to future studies to use a global decreasing coefficient, which includes both processes. Another possible alternative to represent processes is to include the sediment loading that comes from the bottom of the reservoir.

Some other model details can be varied in future studies, in order to check its influence on final results, such as the heat up time, which was selected the period of a year, and the calculation of surface area of the sediments, that was estimated as being two times the water surface area. The seasonal components can also be explored in future studies.

The choice of which model one should use depends on the purpose of the modelling. If the goal is to address specific locals, a 3D model should be used due to the spatial precision. It is worth remembering that this precision is conditioned to the quality of field measurements used as input and calibration data. Zero-dimensional models, however, are useful for pointing out the general concentration dynamics of each sector. For planning and management purposes, such as the Water Quality Classification Framework of waterbodies, the simplified approach is a valuable tool to spare time and resources.

This model created for water resources planning and management is capable of representing the reservoir dynamics for this purpose with reasonable precision. Its use is recommended for the wide number of Brazilian reservoirs that still were not submitted to the Water Quality Framework Process and do not have a large database of water quality monitoring results.

Another potential use for zero-dimensional modelling is the application of this tool in the context of cascading reservoirs, in a way that integrates with a model suitable for rivers. This application would fulfill a gap noticed in river-reservoir integrated studies: the lack of a specific model that includes both environments and properly considers temporal changes.

This research also provided an overview on the Total Maximum Daily Loads use for planning and management despite the Brazilian regulations only focus on concentration standards. Considering the use of synthetic series, the chronological gaps can be fulfilled and the loadings calculation can provide a general indication of the reservoir condition.

6 REFERENCES

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APPENDIX A – Equation for the unsteady flow state, with variable volume

Starting from the equation presented by Chapra (2008):

$$\frac{dc\boldsymbol{V}}{dt} = Q_{in}c_{in} - Q_{out}c_{out} - kVc - v\,A_s c$$

Applying the product rule:

$$V\frac{dc}{dt} + c\frac{dV}{dt} = Q_{in}c_{in} - Q_{out}c_{out} - kVc - v\,A_s c$$

Using the finite difference method:

$$V\frac{(c_{i+1} - c_i)}{\Delta t} + c\frac{\Delta V}{\Delta t} = Q_{in}c_{in} - Q_{out}c_{out} - kVc - v\,A_s c$$

Putting the indices in the equation:

$$V_{i+1}\frac{(c_{out\,i+1} - c_{out\,i})}{\Delta t} + c_{out\,i+1}\frac{(V_{i+1} - V_i)}{\Delta t} = Q_{in\,i+1}c_{in\,i+1} - Q_{out\,i+1}c_{out\,i+1} - kV_{i+1}c_{out\,i+1} - v\,A_{s\,i+1}\,c_{out\,i+1}$$

$$c_{out\,i+1} = c_{out\,i} + \frac{\Delta t}{V_{i+1}}\left(Q_{in\,i+1}c_{in\,i+1} - Q_{out\,i+1}c_{out\,i+1} - kV_{i+1}c_{out\,i+1} - v\,A_{s\,i+1}\,c_{out\,i+1} - c_{out\,i+1}\frac{(V_{i+1} - V_i)}{\Delta t}\right)$$

Isolating the term $c_{out\,i+1}$:

$$c_{out\,i+1} = \frac{c_{out\,i} + \frac{\Delta t}{V_{i+1}}(Q_{in\,i+1}c_{in\,i+1})}{1 + \frac{\Delta t}{V_{i+1}}\left[Q_{out\,i+1} + kV_{i+1} + v\,A_{s\,i+1} + \frac{(V_{i+1} - V_i)}{\Delta t}\right]}$$

The Δt and the ΔV were defined as follows:

$$\Delta t = t_{i+1} - t_i$$

$$\Delta V = V_{i+1} - V_i$$